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AEROTHERMAL MODELING PROGRAM PHASE I FINAL REPORT

by

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Garrett Turbine Engine Company
A Division of The Garrett Corporation

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SECTION I

1.0 SUMMARY

The main objective of the NASA-sponsored Aerothermal Modeling Program, Phase I was to assess current aerothermal submodels used in the Garrett Turbine Engine Company (GTEC) analytical combustor models.

A number of "benchmark" quality test cases were selected after an extensive literature survey. The selected test cases, both nonreacting and reacting flows, were broadly divided into the following categories:

- o Simple flows
- o Complex nonswirling flows
- o Swirling flows
- o Dilution jet mixing in confined crossflows.

These test cases were used to assess the following submodels separately and jointly for various combustion processes:

- k-€ model of turbulence and algebraic stress model, with and without various corrections including low Reynolds number and Richardson number corrections
- o Scalar transport models
- o Multistep kinetic schemes
- o Turbulence/chemistry interaction
- o Spray combustion.

The following general conclusions were derived from Phase I work.

- o An accurate numerical scheme should be developed to minimize numerical diffusion in the computations of recirculating flows
- o Benchmark quality data should be generated under welldefined environments for validating the various submodels used in gas turbine combustion analysis.
- o Although current aerothermal models make reasonable predictions, intensive model development and validation effort should continue for the following submodels:
 - Algebraic stress model
 - Algebraic scalar transport model
 - Two-step and four-step schemes
 - probability density function approach for a twostep scheme
 - Double-reaction zone model.

SECTION II

2.0 INTRODUCTION

The objectives of the NASA Aerothermal Modeling Program are to assess the current state-of-the-art and identify the deficiencies in current aerothermal models for gas turbine combustors. The program involves the following tasks:

Task 1.1 - Model Definition

Task 1.2 - Data Base Generation

Task 1.3 - Benchmark Test Case Definition

Task 2.1 - Model Execution

Task 2.2 - Model Assessment

Task 2.3 - Program Plan for Model Improvement.

Paragraph 2.1 gives a brief background of aerothermal modeling followed by a description of the Garrett empirical/analytical combustor design approach in Paragraph 2.2. This design approach is based on the use of a number of interrelated multidimensional analytical models that contain appropriate submodels (modules) of turbulence, chemistry, spray combustion/evaporation, soot, and high pressure radiation. These modules are described in Section 3.0. A description of the numerical schemes employed are provided in Section 4.0, and a survey of relevant literature is presented in Section 5.0.

The model assessment results are presented in four different sections:

- o Section 6.0 Results for simple flows, with and without combustion
- o Section 7.0 Results for complex nonswirling flows

- o Section 8.0 Evaluation of the models for swirling flows
- o Section 9.0 Three-dimensional (3-D) dilution jetmixing validation results

Section 10.0 presents the conclusions and the recommendations for model improvements.

2.1 Aerothermal Modeling Background

Substantial increases in gas turbine performance have been achieved in recent years due largely to the use of advanced technologies in components and material, in addition to operation at higher cycle pressures and temperatures. To meet the trend toward higher pressure ratio gas turbines with increased turbine inlet temperatures, increased research and development efforts have been directed toward the combustion system. These efforts have contributed largely toward gaining a better understanding of the overall combustion process and have led to the development of an advanced combuster design methodology based on a combination of empirical and analytical techniques. The challenging demands placed upon the combustion system due to increased performance and life requirements, as well as the need to reduce combustor design and development cost, have provided the primary motivation for using multidimensional combustion analysis procedures. The advanced combustion analysis forms the basis for the design and development procedures of advanced technology combustors at Garrett Turbine Engine Company. 1-10

To provide greater confidence in the design of high-performance, durable combustors for advanced aircraft turbine engines, a thorough understanding and accurate characterization of the various physical phenomena involved is required. Over the years, Garrett has been actively involved in the assessment, validation, and updating of combustor aerothermal models in the areas of multidimensional flow effects, effects of turbulence scale and intensity, combustion kinetics, fuel spray and flow field interactions, soot formation, and high-pressure flame radiation characteristics. Garrett has continued to assess every submodel within each model against fundamental data from ideal element tests. 10-14 Concurrently, model accuracy has been indirectly assessed by comparing predictions with measurements on a number of production and advanced combustors. 1-9 Through an integrated effort of assessing both the models and the submodels, it has been possible to continually improve the accuracy and reliability of the empirical/analytical design procedure described in the following paragraph.

2.2 Garrett Empirical/Analytical Combustor Design Approach

Past approaches to the design and development of gas turbine combustion systems have largely involved the application of fundamental knowledge of turbulent reacting flows on an empirical basis, followed by component testing to achieve optimum performance objectives. A number of semiempirical relationships have been developed through the years to provide guidelines for the initial design of a new combustion system and to predict attainable performance on the basis of experience curves. Such an approach has been quite successful in the design and development of combustor configurations that are derived from proven concepts.

The development of an empirical data base for combustors is evolutionary. Its limitations, regarding the development of advanced combustion systems with requirements outside of experience bounds, became apparent to Garrett in the early 1970's. The inadequacy of the empirical approach in solving combustion development problems relating to gaseous and particulate emissions; carbon formation; and, more recently, liner and nozzle structural durability for high-temperature-rise applications required complementing this approach with advanced analytical methods.

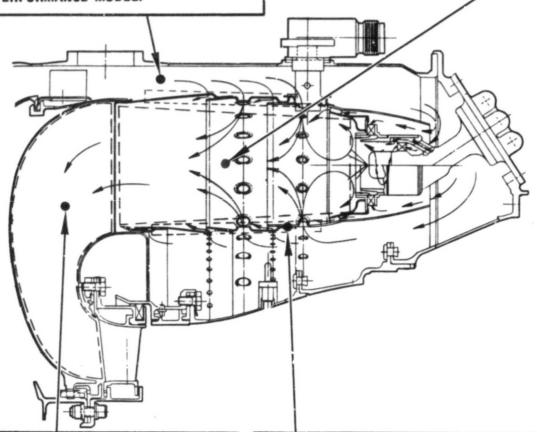
Garrett has developed a number of analytical models that form the basis for the design and development of advanced technology combustors. The internal flow field of modern gas turbine combustors is a highly complex 3-D phenomenon involving regions of reverse-flow. In addition, the various combustor regions require varying degrees of field resolution to predict accurately the convective and radiative fluxes. A modular approach, therefore, has been developed at Garrett allowing use of different computer models, as depicted in Figure 2.2-1.

ANNULUS FLOW MODEL, AFM

SOLVES FOR THE PRESSURE LOSSES AND AIRFLOW DISTRIBUTION WITHIN THE ANNULUS EXTERNAL TO THE COMBUSTOR. PREDICTS THE REQUIRED ORIFICE PATTERN FOR THE DESIRED FLOW SPLITS AND THE BOUNDARY CONDITIONS FOR THE COMBUSTOR PERFORMANCE MODEL.

COMBUSTOR PERFORMANCE MODEL, CPM

SOLVES THE GOVERNING REACTING
FLUID DYNAMIC AND CHEMICAL REACTION
EQUATIONS FOR THE ENTIRE COMBUSTOR.
PREDICTS THE COMBUSTOR-FLOW FIELD
INCLUDING VELOCITIES, TEMPERATURE, AND
LOCAL FUEL-AIR RATIO AS WELL AS SMOKE
AND SPECIES CONCENTRATION.



TRANSITION MIXING MODEL, TMM

SOLVES THE GOVERNING REACTING FLUID DYNAMIC AND CHEMICAL REACTION EQUATIONS IN THE 180° TRANSITION LINER BEND PREDICTS THE TEMPERATURE QUALITY AT THE FIRST-STAGE TURBINE INLET.

NEAR WALL MODEL, NWM

SOLVES THE GOVERNING FLUID DYNAMIC AND HEAT FLUX EQUATIONS ADJACENT TO THE LINER WALLS USING A HIGH-RESOLUTION GRID. PREDICTS LINER HEAT TRANSFER RATES AND ATTENDANT WALL TEMPERATURES.

Figure 2.2-1 Combustor Models and Region of Application.

An annulus flow model is used to calculate pressure losses and airflow distribution within the annulus external to the combustor liner. This model calculates boundary conditions, such as flow distribution around the liner, jet velocity, and efflux angles, which are required as inputs for the combustor internal flow models.

Two-dimensional (2-D) and 3-D combustor performance models are used to predict internal profiles of dependent variables including velocity, species, and temperature by solving fully coupled transport equations for turbulent, recirculating, spray-combusting flow fields. Up to 20,000 finite-difference grid nodes are numerically solved in these programs to ensure a relatively "grid-independent" solution for the main flow field. However, for the region close to the film-cooled wall, a better field resolution is required to accurately predict the convective fluxes and the wall temperatures. This is done by using near-wall models.

The reverse-flow annular combustors generally employ transition liners where the main flow direction changes from axial to radial for radial-inflow turbines or a full 180-degree bend for axial flow turbines. The flow field has only small pockets of reverse-flow regions. Computationally more efficient 2-D and/or 3-D transition mixing models are used for calculating the mixing rate of the cold dilution jets in the transition liner. These models calculate the turbine stator inlet profiles of temperature, velocity, and turbulence intensity, which are needed for assessing turbine hardware life. The various analytical models are used in the overall combustor design to arrive at a final combustor design in a timely and cost-effective manner.

The empirical/analytical combustor design approach is shown in Figure 2.2-2. The engine requirements and design define the combustor inlet conditions and limiting envelope constraints. Using

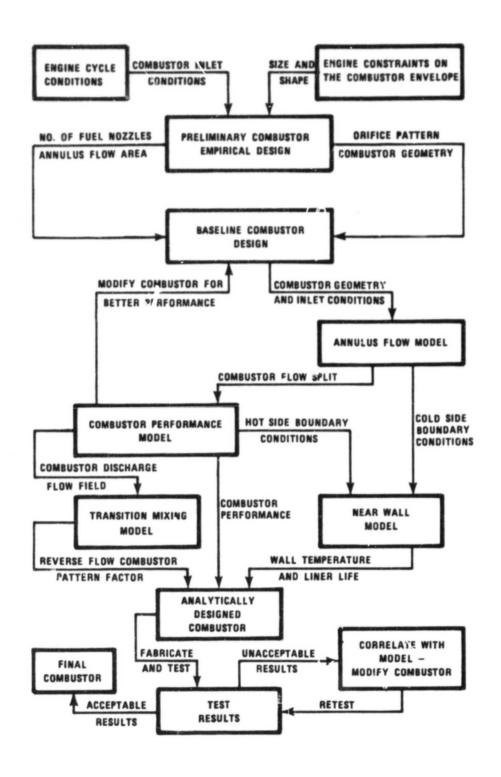


Figure 2.2-2. Comoustor Design Methodology.

existing empirical design relations, a baseline combustor is defined and includes the appropriate flow splits, number of fuel nozzles, and orifice locations. The annulus flow model is then used to determine the orifice sizes to obtain the desired overall pressure drop, and flow splits needed to define the boundary conditions for the combustor performance model.

The combustor performance model is run at various power conditions to evaluate combustor internal flow characteristics. If the design requires changes, the baseline combustor is altered, the annulus flow model is rerun, and the combustor performance model is again used to evaluate the new design.

The combustor liner wall convective and radiative fluxes and attendant temperature levels and gradients are calculated with the near-wall model. The hot-side boundary conditions are defined by the combustor performance model. The cold-side boundary conditions are defined by the annulus flow model. The combustor performance model is also used to define initial conditions for the transition mixing model, which is used to calculate the mixing in the transition liner and the resulting burner exit temperature quality.

The results from the combustor performance model, near-wall model, and transition mixing model are factored into the analytically designed combustor. If the design is lacking, iterations are performed using the various models to arrive at an acceptable final configuration.

The configuration is then fabricated and tested. If the result is unacceptable, the test data is compared with the analytical predictions and the appropriate subcomponent is modified, reanalyzed, and retested to verify that the modifications corrected the problems. This procedure is repeated until all the combustor design goals are achieved. Experience shows that this design

approach minimizes the number of changes required on actual hardware to achieve the design objectives.

SECTION III

3.0 Description of Analytical Models

Detailed descriptions of the combustor analytical models are provided in Paragraph 3.1. Each analytical model contains several submodels, which are described separately in Paragraphs 3.2 through 3.6.

3.1 The Analytical Models

The Garrett modular analytical approach uses the following four models for analyzing gas turbine combustor flow field.

- o Annulus Flow Model (AFM)
- o Combustor Performance Model (CPM), 2-D and 3-D
- o Transition Mixing Model (TMM), 2-D and 3-D
- o Near-Wall Model (NWM)

These models use submodels of turbulence, kinetics, radiation, and spray combustion/evaporation and dispersion as summarized in Table 1.

3.1.1 Annulus Flow Model

The first task in analyzing any combustion system is to predict the annulus flow external to the combustor. For this, the AFM is used. The combustor annulus is divided into a number of sections with the section boundaries defined by orifice rows in the liner or points of significant area change. In each section, the AFM solves the one-dimensional (1-D) equations for axial and tangential velocity. Mass is extracted from the annulus flow at each orifice row. The extracted mass is governed by the liner orifice

TABLE 1. COMPUTER MODELS AND PHYSICAL SUBMODELS (MODULES).

			SUBMODELS (MODULES)					
MODEL	DIMEN- SIONS	NUMERICAL TYPE	TURBU- LENCE	KINETICS	RADIA- TION	SPRAY	INPUTS INFO TO:	OBTAINS INFO FROM:
ANNULUS FLOW (AFM)	1	-	-	-	-	-	СРМ	-
COMBUSTOR PERFORMANCE (CPM)	2/3	ELLIPTIC; ORTHOGONAL/ NONORTHOGONAL	K-e	2-STEP/ 4-STEP	4-FLUX/ 6 FLUX	LAGHANGIAN AND/OR EULERIAN	TMM NWM	AFM
TRANSITION MIXING (TMM)	2/3	PARABOLIC/ ELLIPTIC; NONORTHOGONAL	K-€	2-STEP	NONE/ 6 FLUX	NONE	-	СРМ
NEAR WALL (NWM)	1/ 2/ 3	PARABOLIC/ ELLIPTIC	K-€	2-STEP	2-FLUX	NGNE	-	СРМ

geometry and semi-analytical correlations for discharge coefficient. Pressure loss, both frictional and dump types, and heat transfer are included in the calculations. Iteration on combustor liner pressure drop continues until the total orifice flow rate achieves the desired value. The AFM predicts the static pressure distribution around the combustor, the liner pressure drop, orifice flow splits, and injection angles and velocities. These values are required as boundary conditions for the internal combustor flow programs (CPM, TMM, and NWM).

3.1.2 Combustor Performance Model

The CPM has two versions: 2-D and 3-D.

2-D Combustor Performance Model

If the internal flow field of the combustor is predominantly 2-D plane flow or axisymmetric flow, a 2-D CPM is used to calculate combustor internal flow field. The 2-D CPM is a generalized finite-difference program that solves the conservative form of the the governing fluid dynamic and chemical reaction equations, using the numerical scheme of Patankar-Spalding. The following variables are solved:

- o Axial, radial, and tangential velocity
- o Turbulent kinetic energy and dissipation
- o Total fuel, unburned fuel, and other chemical species including carlon monoxide
- o Pressure
- o Stagnation enthalpy

- o Radiation
- o Liquid particle droplet size, velocity, and evaporation rate

Cylindrical or rectangular coordinates are used along with the capability of specifying any arbitrary shape for the liner wall or any arbitrary internal object such as a fuel nozzle shroud. Using the flow rates and velocities, etc., from the AFM, cooling slots, primary and dilution orifices, swirlers, and liquid or gaseous fuel nozzles are all modeled simultaneously. This gives the overall combustor flow field and the species and temperature distributions. Bulk flow properties determined include recirculation zone size and shape, primary and dilution jet penetration, and combustion efficiency.

3-D Combustor Performance Model

In many situations, the combustor geometry is not 2-D. In these cases, 3-D CPM must be used. The 3-D CPM is based on the USARTL 3-D Model¹² and can be considered an extension of the 2-D CPM to three dimensions. Both models use the same numerical scheme and the coordinate system. Like the 2-D CPM, the 3-D CPM solves for similar variables and requires boundary condition input from the AFM. Arbitrary complex boundaries and nozzle shrouds can be simulated. The 3-D CPM can analyze such 3-D flow situations as single (or multiple) swirlers in an annular combustor, tangential fuel nozzles, and discrete primary and dilution jets.

3.1.3 Transition Mixing Model

The TMM has two versions: 2-D and 3-D.

2-D Transition Mixing Models

Though the 2-D CPM and 3-D CPM can analyze arbitrary shapes, they are limited to cylindrical or Cartesian coordinates. cannot economically calculate the flow in the transition liner used in reverse-flow annular combustion systems. For relatively long combustors where the flow entering the transition liner is predominantly 2-D, the 2-D transition mixing model (2-D TMM) is used. This model is based on the GENMIX program of Patankar and ${\tt Spalding}^{{\tt l6}}$. Modifications have been added that allow the program to negotiate 180-degree bends with the source terms added to account for the induced radial pressure gradients. Since it is a parabolic numerical scheme, this model is limited to transition liners in which the radii of curvature are large. Otherwise the pressure effects would have to propagate upstream. As in the other Garrett models, the two-equation $k-\epsilon$ turbulence model is used along with the 2-step reaction mechanism. For initial profiles, the 2-D TMM uses the exit profiles as predicted by either the 2-D CPM or 3-D CPM. It then generates the exit profiles from the transition liner to which the turbine stator is exposed.

3-D Transition Mixing Models

With current trends toward shorter turbo-propulsion combustors and more compact transition liners, a significant amount of dilution jet mixing and spreading takes place within the transition liner. Attendant 3-D flow characteristics result from this mixing and spreading. Moreover, due to tight-bend radii of the transition liner, upstream (elliptic) effects caused by streamline curvature cannot be ignored.

A 3-D elliptic transition mixing model has therefore been developed that includes radiation and kinetic effects on the transition liner. This program is similar to the 3-D CPM, but has been structured to afford more than 2000 L finite-difference

nodes, where L is the number of nodes along the predominant flow direction. Theoretically, there is no limit on L; however, due to computer time consideration, L is generally kept less than 50. The 3-D TMM can be adopted to analyze turbopropulsion combustors with much more complex geometries that cannot be adequately discretized by a cylindrical or Cartesian coordinate system.

3.1.4 Near-Wall Models

To accurately predict hot-side convective and radiative fluxes to the liner wall, a 2-D parabolic film cooling analytical model was developed during the Army Combustor Design Criteria Program. Subsequently, an improved 2-D NWM has been developed to allow a more accurate assessment of the effects of the following on liner cooling effectiveness:

- o Slot geometry
- o Primary/dilution jets
- o Flow in the lateral directions
- o Radiation from the bulk flow field and the opposite wall
- o Spray combustion adjacent to the wall.

The 2-D NWM can be used interactively with the combustor performance models to more accurately predict near-wall flow field. The 2-D NWM uses the same modules as the CPM.

To further improve near-wall calculations, 2-D elliptic and 3-D parabolic NWM have also been developed at Garrett.

3.2 Description of Turbulence and Scalar Transport

The internal flow field in gas turbine combustors is highly turbulent and recirculating. Efficient design of combustion systems requires a detailed understanding of the physic-chemical processes of such systems. A prerequisite for this understanding is an ability to analyze the nonreacting turbulent recirculating flows.

The fluid dynamics of turbulent flows are governed by the time-dependent Navier-Stokes equations. Solutions of these equations are extremely difficult and require prohibitively large computational time. Furthermore, subgrid models are required to describe the transport phenomena in addition to the Navier-Stokes equations. A common alternative is to use time-averaged Navier-Stokes equations. This system of equations contains unknown higher order correlations resulting in a greater number of unknowns than the number of available equations. Turbulence models of the higher order correlations based on phenomenological assumptions are needed to close this system of equations. The degree of success of a turbulence model depends on the nature and accuracy of the phenomenological assumptions.

The simplest of the turbulence models are the mixing-length models. In these models, the characteristic length scales of turbulence are often prescribed to close the system of equations. These models have been successful in treating simple flows like boundary layers and pipe flows, but have been unsuccessful in analyzing recirculating flows.

The next higher order turbulence models are the one-equation models. These models solve one differential equation for determining the distribution of the turbulent kinetic energy or equivalent characteristic property of turbulence. The characteristic

length scale is defined in a manner similar to mixing-length models. Consequently, the one-equation models have also been unsuccessful in predicting turbulent recirculating flows.

The two-equation models are more complex than the mixing length models. These models use two differential equations for computing characteristic velocity and length scales. Among the two-equation models, the $k-\epsilon$ model has been the most successful so far. The $k-\epsilon$ model is used in the Garrett combustor analytical models and is described in Paragraph 3.2.1. In regions adjacent to walls, the viscous effects play a prominent role. To provide an accurate prediction of the flow in these regions, a low Reynolds number version of the $k-\epsilon$ model is used in the Garrett near-wall models. This model is described in Paragraph 3.2.2.

Even though the $k-\epsilon$ model has been the most successful in predicting recirculating flows, the predictions for flows with streamline curvatures have been only qualitatively correct. Flow fields involving streamline curvatures have been known to have increased turbulence diffusion rates due to enhanced turbulence production. This increased turbulence production is not adequately accounted for in the $k-\epsilon$ model. One way to include this extra production of turbulence is to modify the constants in the $k-\epsilon$ model in proportion to the Richardson number, which is a measure of the extra strain rate produced by the streamline curvature. These corrections are described in Paragraph 3.2.3.

The Richardson number corrections are applicable for flows with moderate streamline curvature effects. For flows with strong curvature effects, a solution of the Reynolds stress equations is necessary. Solution of the complete Reynolds stress components results in increased computational time. An attractive alternative is the use of an algebraic Reynolds stress model. In this model,

the terms in the Reynolds stress transport equations are approximated to yield algebraic expressions in terms of the turbulence kinetic energy and length scale. The degree of approximations employed would determine the accuracy of predictions. The algebraic Reynolds stress model is described in Paragraph 3.2.4.

In complex combustor flow fields, the approximations used in developing the algebraic Reynolds stress model are not valid. For such flow fields, the Reynolds stress components must be obtained from the solution of differential transport equations for the appropriate Reynolds stress component. A description of these equations used by Garrett are provided in Paragraph 3.2.4.

Another important submodel for combustor internal flows is the scalar transport model. The accuracy of the combustor performance predictions depends upon the accuracy of predicting the transport of scalar properties such as concentration of reactants, etc. The most commonly used scalar transport model is the gradient diffusion model. The gradient diffusion model does not adequately account for counter-gradient transport, which has been known to exist in most combustor internal flow fields. An algebraic scalar transport model (ASTM) has been developed at Garrett, which can predict counter-gradient scalar transport. This model is described in Paragraph 3.2.2.

3.2.1 Governing Equations for the $k-\epsilon$ Model

The time-averaged transport equations for turbulence kinetic energy (k) and its dissipation rate (ϵ) can be written in the following generalized variable form:

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$$\frac{1}{r} \left\{ \frac{\partial}{\partial x} \left(\rho r \cup \phi \right) + \frac{\partial}{\partial r} \left(\rho r \vee \phi \right) + \frac{\partial}{\partial \theta} \left(\rho \vee \phi \right) \right.$$

$$- \frac{\partial}{\partial x} \left(r \Gamma_{\text{eff}}, \phi \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial r} \left(r \Gamma_{\text{eff}}, \phi \frac{\partial \phi}{\partial r} \right)$$

$$- \frac{1}{r} \left. \frac{\partial}{\partial \theta} \left(\Gamma_{\text{eff}}, \phi \frac{1}{r} \frac{\partial \phi}{\partial \theta} \right) \right\} = S_{\phi} \tag{1}$$

Here ρ , $\Gamma_{\rm eff}$, ϕ and S_{ϕ} denote the fluid density, the local effective exchange coefficient of variable ϕ , and sources/sinks. The source terms for the dependent variables are

Turbulence kintetic energy,
$$k = \frac{1}{2}(\overline{u^2} + \overline{v^2} + \overline{w^2})$$

$$S_k = G_k - \rho \epsilon \qquad (2)$$

where

$$G_{\mathbf{k}} = \mu_{\dagger} \left[2 \left\{ \left(\frac{\partial U}{\partial x} \right)^{2} + \left(\frac{\partial V}{\partial r} \right)^{2} + \left(\frac{1}{r} \frac{\partial W}{\partial \theta} + \frac{V}{r} \right)^{2} \right.$$

$$\left. + \left(\frac{\partial W}{\partial x} + \frac{1}{r} \frac{\partial U}{\partial \theta} \right)^{2} + \left(\frac{\partial U}{\partial r} + \frac{\partial V}{\partial x} \right)^{2} \right.$$

$$\left. + \left(\frac{\partial W}{\partial r} + \frac{1}{r} \frac{\partial V}{\partial \theta} - \frac{W}{r} \right)^{2} \right]$$
(3)

o Dissipation rate,

$$S_{\epsilon} = (C_1 G_k - C_2 \rho_{\epsilon}) \frac{\epsilon}{k}$$
(4)

The effective viscosity is obtained from the relation

$$\mu_{eff} = \mu + \mu_{t}$$

where μ and $\mu_{\rm t}$ are the molecular and turbulent viscosities, respectively. $\mu_{\rm t}$ is related to k and ϵ via

$$\mu_t = C_D \rho k^2 / \epsilon$$
 (5)

The exchange coefficients are defined as

$$\Gamma_{\rm eff,}\phi = \mu_{\rm eff}/\sigma_{\rm eff,}\phi$$

Recommended values for the constants in the above equations are

$$C_{D} = 0.09$$
 $C_{1} = 1.44$
 $C_{2} = 1.92$
 $C_{eff} = 0.9$

 $\sigma_{ ext{eff, }\epsilon}$ is calculated from

$$\sigma_{\text{eff},\epsilon} = \frac{\kappa^2}{(C_2 - C_1) C_D^{1/2}}$$
(6)

where the K is the von Karman constant taken to be 0.41.

The near-wall region is given a special treatment in the program. Since the expression for $\Gamma_{\rm eff}$ is accurate for turbulent flows only, a means is provided for the inclusion of the correct shear stresses and other fluxes at the wall. Therefore, the nodes next to the wall are assigned the following values as per an empirical wall law:

$$y^{+} \leq 11.5 \qquad \Gamma_{\phi,\text{wall}} = \frac{\mu}{\sigma \phi}$$

$$y^{+} > 11.5 \qquad \Gamma_{\phi,\text{wall}} = \frac{\mu}{\sigma \phi} \frac{y^{+}}{\frac{1}{\kappa} \ln(9y^{+}) + P_{\phi}}$$
(7)

$$y^{+} = \rho k^{1/2} C_{D}^{1/4} \frac{\delta}{\mu}$$

$$P_{\phi} = 9.0 \left(\frac{\sigma}{\sigma_{\text{eff}}} - 1\right) \left(\frac{\sigma}{\sigma_{\text{eff}}}\right)^{-1/4}$$
(8)

where δ is the normal distance of the wall from the first interior adjacent node and σ is the laminar Schmidt number.

The kinetic energy of turbulence has small diffusion near the wall; hence, Γ_{wall} for k is set equal to zero. Instead of computing Γ_{wall} for ϵ , it is calculated for the near-wall node by assuming a linear variation of the length scale giving the following expression:

$$\epsilon = C_D^{3/4} k^{3/2} / (\kappa \delta) \tag{9}$$

3.2.2 Near-Wall Low Reynolds Number Correction

In the near-wall region, the wall function approach, described in the previous paragraph does not properly describe the behavior of Eurbulence kinetic energy and its dissipation rate. A systematic Taylor Series expansion technique has been developed by Chien, 17 which correctly describes the turbulent shear stresses, kinetic energy, and its dissipation rate in the region near a wall. To maintain the consistency of the behavior of k and ϵ near the

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wall, additional terms had to be added to the k and ϵ equations and the turbulent effective diffusion rates were modified. The corrected equations of Chien near the wall are as follows:

Turbulence kinetic energy; k

$$\frac{\partial}{\partial x} (\rho \dot{U} k) + \frac{1}{r} \frac{\partial}{\partial r} (\rho r V k) = \frac{\partial}{\partial x} \left(\Gamma_{eff,k} \frac{\partial k}{\partial x} \right)$$

$$+ \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{eff,k} \frac{\partial k}{\partial r} \right] + S_k + D$$
(10)

where, D is the extra source term, given by

$$D = -2\mu \frac{k}{y^2} \tag{11}$$

$$\Gamma_{\text{eff,k}} = (\mu + \mu_{\text{t}} f_{\mu})/\sigma_{\text{eff,k}}$$
 (12)

$$f_{\mu} = 1.0 - \exp(-0.0115 \, y^{+})$$
 (13)

 S_k is the source term described in equation (2)

Dissipation Rate, ϵ

$$\frac{\partial}{\partial x} (\rho U \epsilon) + \frac{1}{r} \frac{\partial}{\partial r} (r \rho V \epsilon) = \frac{\partial}{\partial x} \left[\Gamma_{\text{eff}, \epsilon} \frac{\partial \epsilon}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \Gamma_{\text{eff}, \epsilon} \frac{\partial \epsilon}{\partial r} \right] + S_{\epsilon} + E$$
(14)

where, E is the additional source term for dissipation, defined as

$$E = -2 \mu \exp(-0.5 y+) \frac{\epsilon}{y^2}$$
 (15)

and
$$S_{\epsilon} = (C_1 G_k - C_2 f_2 \rho \epsilon) \frac{\epsilon}{k}$$
 (16)

with
$$f_2 = 1.0 - 0.22 \exp(-R_{7}/6)^2$$
 (17)

$$R_T = \frac{\rho k^2}{\mu \epsilon}$$

In the modified k and ϵ equations, it is possible to apply the boundary conditions at the wall, with k = 0 and ϵ = 0 at y = 0. This approach gives consistent results near the wall.

3.2.3 Richardson Numbers Correction to $k-\epsilon$ Model

The standard $k-\epsilon$ model presented in Paragraph 3.2.1 describes the turbulence characteristics at any point in the flow field by a single velocity and length scale. These scales are obtained from an assumed isotropic turbulence structure. This model is adequate for simple flow fields. When significant streamline curvatures are introduced into the flow field, such as strong recirculation zones or swirl, the $k-\epsilon$ model does not adequately account for the enhanced turbulence diffusion caused by the extra strain rates associated with streamline curvature. For analyzing such flow fields, the $k-\epsilon$ model should be modified.

A measure of the extra strain rate due to the streamline curvature is given by the Richardson number, Ri. The extra strain rate imposed on the flow field would tend to increase both the velocity and the length scales of turbulence. One way to account for the changes in the characteristic scales is to modify the turbulence

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constants depending upon the Richardson number. For 2-D recirculating flows, the Richardson number can be defined as

$$Ri_{c} = \frac{k^{2}}{\epsilon^{2}} \frac{V_{R}}{R^{2}} \frac{\partial}{\partial R} (RV_{R})$$
 (18)

where, V_R and R are the resultant velocity and the radius of curvature respectively. They are defined as

$$V_{R} = \sqrt{U^2 + V^2} \tag{19}$$

$$\frac{1}{R} = \frac{UV(\frac{\partial V}{\partial y} - \frac{\partial U}{\partial x}) + U^2 \frac{\partial V}{\partial x} - V^2 \frac{\partial U}{\partial y}}{V_R^3}$$
(20)

For swirling flows, the corresponding Richardson number is defined by

$$Ri_{V_{\theta}} = \frac{\left(\frac{V_{\theta}}{r^2}\right) \frac{\partial}{\partial r} (r V_{\theta})}{\left(\frac{\partial U}{\partial r}\right)^2 + \left(r \frac{\partial}{\partial r} \left[\frac{V_{\theta}}{r}\right]\right)^2}$$
(21)

In the $k-\epsilon$ model, the governing equation for k is an exact equation and no empirical modeling is involved in it. However, the ϵ equation is a modeled equation containing two empirical constants. The adopted approach is to modify the constant C_2 in the equation by the following expression

$$C_2 = 1.92 \exp \left(-\alpha_{V_{\theta}} \operatorname{Ri}_{V_{\theta}} - \alpha_{c} \operatorname{Ri}_{c}\right). \tag{22}$$

Here $\alpha_{V\theta}$ and α_{C} are empirical constants, whose values are of the order of 0.2.

3.2.4 Algebraic Reynolds Stress Model

Turbulent flow fields occurring in combustors are generally nonisotropic in character. The turbulent diffusion rates in different directions are different depending upon the strain-rate tensor. Descriptions of such flow fields necessitate knowledge of the complete Reynolds stress components. Solution of the complete Reynolds stress components is expensive and complex. An alternative to this approach is the algebraic Reynolds stress model.

The algebraic Reynolds stress model is obtained by approximating some of the higher order terms in the Reynolds stress equation based upon phenomenological simplifications. The approximations result in algebraic expressions for the Reynolds stress components with added empirical constants.

The exact transport equation for Reynolds stress $\overline{u_iu_j}$ at high Reynolds numbers in an incompressible flow can be written in the form

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$$\underbrace{\frac{D}{Dt} \left(\overline{u_i u_j} \right)_{=} - \frac{\partial}{\partial x_k} \left(\overline{u_k u_i u_j} \right) - \frac{1}{\rho} \left(\frac{\partial \overline{u_j p'}}{\partial x_i} + \frac{\partial \overline{u_j p'}}{\partial x_j} \right) - 2 \frac{\mu}{\rho} \left(\frac{\partial \overline{u_i}}{\partial x_k} - \frac{\partial \overline{u_j}}{\partial x_k} \right)}_{\text{Convection}}$$

$$- \left(\underbrace{\overline{u_i u_k}}_{ij} \frac{\partial \overline{u_j}}{\partial x_k} + \underbrace{\overline{u_j u_k}}_{ij} \frac{\partial \overline{u_j}}{\partial x_k} \right) + \underbrace{\frac{p'}{\rho} \left(\frac{\partial \overline{u_j}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i} \right)}_{\pi_{ij} = \text{Pressure-Strain}} \tag{23}$$

At high Reynolds numbers, the viscous dissipation ϵ_{ij} is essentially due to the small scale turbulent motions and hence tends to isotropize $\overline{u_i u_j}$. The pressure-strain term has been modeled by Rodi in the form

$$\pi_{ij} = \pi_{ij,1} + \pi_{ij,2} \tag{24}$$

 $\pi_{ij,l}$ represents the contributions to pressure strain arising from fluctuating velocities only, and $\pi_{ij,2}$ accounts for the interactions between fluctuating velocities and mean strain. These terms are modeled as follows:

$$\pi_{ij,l} = -C'_{l} \frac{\epsilon}{k} \left[\overline{\nu_{i}\nu_{j}} - \frac{2}{3} \delta_{ij} k \right]$$
 (25)

$$\pi_{ij,2} = -\alpha \left(P_{ij} - \frac{2}{3} P \delta_{ij} \right) - \beta \left(D_{ij} - \frac{2}{3} P \delta_{ij} \right) - \gamma k \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)$$
 (26)

where:

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$$C'_{1} = 1.5, \ \alpha = \frac{8 + C'_{2}}{11}, \ \beta = \frac{8 C'_{2} - 2}{11}$$

$$\gamma = \frac{30 \text{ C'}_2 - 2}{55}$$
, and $\text{C'}_2 = 0.5$

$$p_{ij} = -\left(\frac{\partial U_i}{\partial x_k} + \frac{\partial U_j}{\partial x_k} + \frac{\partial U_i}{\partial x_k}\right)$$
 (27)

$$D_{ij} = -\left(\frac{\overline{v_i v_k}}{\partial x_j} + \frac{\partial^U k}{\partial x_j} + \frac{\partial^U k}{\partial x_i}\right)$$
 (28)

Rodi has proposed that the convection and diffusion of $\overline{u_i u_j}$ can be scaled by

$$\frac{D}{D_{t}} \overline{(v_{i}v_{j})} - Diff \overline{(v_{i}v_{j})} = \frac{\overline{v_{i}v_{j}}}{k} \left\{ \frac{Dk}{D_{t}} - Diff(k) \right\}$$

$$= \frac{\overline{v_{i}v_{j}}}{k} (P - \epsilon)$$

With this simplification, the above equation reduces to the form

$$\frac{\overline{U}^{2}}{\overline{U}^{2}} = \frac{\frac{2}{3} \epsilon \left(C_{1}^{'} - I\right) + \frac{2}{3} P \left(\alpha + \beta\right) + 2 \left(I - \alpha\right) P}{C_{1}^{'} \frac{\epsilon}{k} + C_{U'} \frac{P - \epsilon}{k}}$$
(30)

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$$\frac{\sqrt{2}}{\sqrt{2}} = \frac{\frac{2}{3} \epsilon \left(C'_{1} - 1\right) + \frac{2}{3} P \left(\alpha + \beta\right) - 2 P\beta}{C'_{1} \frac{\epsilon}{k} + C'_{v} \frac{P - \epsilon}{k}}$$
(31)

$$w^{2} = (2k - v^{2} - v^{2})$$
 (32)

$$-\overline{UV} = \left[\frac{(1-\alpha)\frac{\overline{V^2}}{k} + \gamma - \beta \frac{\overline{U^2}}{k}}{C'_1} \right] \frac{k^2}{\epsilon} \frac{\partial U}{\partial r}$$
 (33)

$$-\overline{vw} = \left\{ (1 - \alpha) \left(\overline{v^2} \frac{\partial V_{\theta}}{\partial r} - \overline{w^2} \frac{V_{\theta}}{r} + \overline{uv} \frac{\partial V_{\theta}}{\partial x} \right) + \gamma k \frac{\partial V_{\theta}}{\partial r} + \beta \left(\overline{v^2} \frac{V_{\theta}}{r} - \overline{w^2} \frac{\partial V_{\theta}}{\partial r} - \overline{uw} \frac{\partial U}{\partial r} \right) \right\} / C'_{1} \frac{\epsilon}{k}$$
(34)

$$-\overline{uw} = \left\{ (1-\alpha) \left(\overline{u^2} \frac{\partial V_{\theta}}{\partial x} + \overline{uv} \frac{\partial V_{\theta}}{\partial r} \right) - \beta \left(\overline{w^2} \frac{\partial V_{\theta}}{\partial x} - \overline{uv} \frac{V_{\theta}}{r} \right) - \gamma k \frac{\partial V_{\theta}}{\partial x} \right\} / C_1' \frac{\epsilon}{k}$$
(35)

From Equation (33):

$$C_{D} = \left[(1 - \alpha) \frac{\overline{v^{2}}}{k} + \gamma - \beta \frac{\overline{v^{2}}}{k} \right] / C'_{1}$$
 (36)

The ASM provides a mechanism by which anisotropic turbulence structure can be predicted without substantial increase in computational effort. The empirical constants in the ASM have not been fully established. They have to be determined by comparing the predictions with the data base.

3.2.5 Reynolds Stress Transport Model

Although the algebraic Reynolds stress model provides a means of computing the anisotropic structure of turbulence, its accuracy in complex turbulent flows is not expected to be good. In the algebraic Reynolds stress model, the closure of the system of equations for Reynolds stresses was achieved by using a scaling law through which the higher order correlations were expressed as functions of lower order correlations. In complex internal combustor flows, the validity of the scaling laws is questionable. In such cases, the only recourse available is to use the Reynolds stress transport model, where the Reynolds stress components are determined by solving modeled differential transport equations for each stress component. The closure of these transport equations was achieved by modeling the higher order correlation terms in a manner analogous to the methods used in the $k-\epsilon$ model.

The governing equations for the Reynolds stress components can be written in generalized form as follows:

$$\frac{1}{r} \left\{ \frac{\partial}{\partial x} (\rho r \cup \phi) + \frac{\partial}{\partial r} (\rho r \vee \phi) + \frac{\partial}{\partial \theta} (\rho \psi \phi) - \frac{\partial}{\partial x} (r \Gamma_{\text{eff}}, \phi \frac{\partial \phi}{\partial x}) - \frac{\partial}{\partial r} (r \Gamma_{\text{eff}}, \phi \frac{\partial \phi}{\partial r}) - \frac{1}{r} \frac{\partial}{\partial \theta} (\Gamma_{\text{eff}}, \phi \frac{1}{r} \frac{\partial \phi}{\partial \theta}) \right\} = S_{\phi}$$
(37)

Here ρ , $\Gamma_{\rm eff,\phi}$ and S_{ϕ} represent the fluid density, local effective exhange coefficient, and the source term for the dependent variable, ϕ . The source terms are

c Axial turbulence normal stress, $\frac{1}{u^2}$

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$$S_{\frac{1}{\sqrt{2}}} = \frac{2}{3} \rho \epsilon (C'_{1} - 1) + \frac{2}{3} G_{k} (\alpha + \beta) - 2 (1 - \alpha) \rho_{\frac{1}{\sqrt{2}}} \frac{\partial U}{\partial r} + 2 \rho_{\frac{1}{2}} \left[\overline{UV} \frac{\partial V}{\partial x} + \overline{UW} \frac{\partial V}{\partial x} \right] - 2 \gamma \rho_{k} \frac{\partial U}{\partial x}$$

$$-2\rho_{\frac{1}{2}} \frac{\partial U}{\partial x} (1 - \alpha - \beta) - C'_{1} \rho_{\frac{1}{2}} \frac{\epsilon}{\sqrt{2}}$$
(38)

Radial Turbulence normal stress,
$$\frac{2}{v^2}$$

$$S_{\frac{1}{\sqrt{2}}} = \frac{2}{3} \rho \epsilon (C_{1} - 1) + \frac{2}{3} G_{k}(\alpha + \beta) -2 \gamma \rho_{k} \frac{\partial V}{\partial r}$$

$$-2 \rho (1 - \alpha) \left[\overline{vv} \quad \frac{\partial V}{\partial x} - \overline{vw} \quad \frac{V_{\theta}}{r} \right]$$

$$+2 \rho \beta \left[\overline{vv} \quad \frac{\partial U}{\partial r} - \overline{vw} \quad \frac{\partial V_{\theta}}{\partial r} \right]$$

$$-C'_{1}\frac{\epsilon}{k}\rho\sqrt{2}-2(1-\alpha-\beta)\rho\sqrt{2}\frac{\partial V}{\partial r}$$
 (39)

o Turbulence Shear Stress, uv

$$S_{\overline{UV}} = -\rho (I - \alpha) \left[\overline{v^2} \quad \frac{\partial U}{\partial r} - \overline{Uw} \quad \frac{V_{\theta}}{r} + \overline{u^2} \quad \frac{\partial V}{\partial x} \right]$$

$$+ \rho \beta \left[\overline{v^2} \quad \frac{\partial V}{\partial x} + \overline{vw} \quad \frac{\partial V_{\theta}}{\partial x} + \overline{uw} \quad \frac{\partial V_{\theta}}{\partial r} + \overline{u^2} \quad \frac{\partial U}{\partial r} \right]$$

$$-\rho\gamma k \left(\frac{\partial U}{\partial r} + \frac{\partial V}{\partial x}\right) + \rho \overline{uv} \frac{V}{r}(1 - \alpha - \beta) - C'_{1} \frac{\rho_{\epsilon}}{k} \overline{uv}$$
 (40)

o Turbulence Shear Stress, www

$$S_{\overline{vw}} = -\rho(1-\alpha) \left[\sqrt{2} \frac{\partial V_{\theta}}{\partial r} - \sqrt{2} \frac{V_{\theta}}{r} + \overline{vv} \frac{\partial V_{\theta}}{\partial x} + \overline{vw} \frac{\partial V}{\partial x} \right]$$

$$+ \rho \beta \left[\overline{w^{2}} \frac{\partial V_{\theta}}{\partial r} + \overline{vw} \frac{\partial U}{\partial r} - \overline{v^{2}} \frac{V_{\theta}}{r} \right] - \rho \gamma k \frac{\partial V_{\theta}}{\partial r}$$

$$+ \rho \overline{vw} \frac{\partial U}{\partial v} (1-\alpha-\beta) - C_{1}^{'} \frac{\rho \epsilon}{k} \overline{vw}$$

$$(41)$$

o Turbulence shear stress, uw

$$S_{\overline{UW}} = -\rho(1-\alpha) \left[\overline{vW} \frac{\partial U}{\partial r} + \overline{u^2} \frac{\partial V_{\theta}}{\partial x} + \overline{uV} \frac{\partial V_{\theta}}{\partial r} \right]$$

$$+ \rho \beta \left[\overline{vW} \frac{\partial V}{\partial x} + \overline{w^2} \frac{\partial V_{\theta}}{\partial x} - \overline{uV} \frac{V_{\theta}}{r} \right]$$

$$- \rho \gamma k \frac{\partial V_{\theta}}{\partial x} - C_{1}^{\prime} \frac{\rho \epsilon}{k} \overline{uW} + \rho \overline{uW} (1-\alpha-\beta) \frac{\partial V}{\partial r}$$

$$(42)$$

Here, C_1 , α , β , and γ are empirical constants, whose values are defined in Equation 26.

Solutions obtained from these equations are used in the momentum equations instead of using the gradient diffusion assumptions. In the new-wall region, boundary conditions for the dependent Reynolds stress components are applied by assuming the convection and diffusion terms to be small, in accordance with the wall function approach. The Reynolds stress component $\overline{w^2}$ is computed from the relation

$$\overline{\mathbf{w}^2} = 2\mathbf{k} - \overline{\mathbf{u}^2} - \overline{\mathbf{v}^2}$$

3.2.6 Scalar Transport Model

The turbulent transport of Scalar properties in a flow is quite different from the transport of momenta. The most common method of describing turbulent scalar transport is the gradient transport law through the use of Prandtl/Schmidt numbers. This apprach is adopted in the standard $k-\epsilon$ model. In the gradient transport model, the turbulent transport parameters of interest are defined by the following.

$$\rho \overline{\cup \theta'} = -\Gamma_{\text{eff}, \theta} \frac{\partial \overline{\theta}}{\partial x}$$
 (43)

$$\rho \overline{\vee \theta'} = - \Gamma_{\text{eff}, \theta} \frac{\partial \overline{\theta}}{\partial r}$$
 (44)

$$\rho \overline{\theta^{,2}} = \frac{2}{\alpha_{\theta}} \frac{k}{\epsilon} \Gamma_{\text{eff}, \theta} \left[\left(\frac{\partial \overline{\theta}}{\partial x} \right)^{2} + \left(\frac{\partial \overline{\theta}}{\partial r} \right)^{2} \right]$$
 (45)

where

$$\Gamma_{\text{eff},\theta} = {}^{\mu}_{\text{eff}}/{}^{\sigma}_{\theta}$$

Here, $^\sigma\!_\theta$ is the Prandtl/Schmidt number for the scalar, θ and $^\alpha\!_\theta$ is an empirical constant. Recommended values for these are, $^\sigma\!_\theta$ = 0.9 and $^\alpha\!_\theta$ = 0.8

The gradient diffusion model does not predict any countergradient diffusive transport. However, in many flows, regions of counter-gradient diffusive transport have been known to exist. For such flows, the scalar transport terms must be obtained from appropriate transport equations.

3.2.7 Algebraic Scalar Transport Model

The governing equations for scalar transport are coupled nonlinear differential equations, which are quite time consuming to However, by using scaling laws analogous to the method used in developing the ASM, it is possible to obtain algebraic expressions for the scalar transport correlations. These expressions could still account for the counter-gradient scalar transport. The detailed steps used in deriving the algebraic scalar transport terms are described in this paragraph.

Transport Equations for
$$u_j\theta'_j$$

Div $(\rho v u_j\theta')$ - Diff $(\rho u_j\theta')$ = $\rho P_j\theta$ - $\rho \epsilon_j\theta$ + $\rho \psi_j\theta$ (46)

Convection Diffusion Production Redistribution

Dissipation

$$P_{j\theta} = - \overline{u_i u_j} \frac{\partial \overline{\theta}}{\partial x_i} - \overline{u_i \theta'} \frac{\partial U_j}{\partial x_j}$$
 (47)

$$\epsilon_{j\theta} = \mu_{eff} \left(\frac{\partial u_j}{\partial x_i} \frac{\partial \theta'}{\partial x_i} \right)$$
(48)

$$\psi_{j\theta} = -C_{l\theta} \frac{\epsilon}{k} \overline{v_{j}\theta'} + c_{2\theta} \overline{v_{i}\theta'} \frac{\partial V_{j}}{\partial x_{j}}$$
(49)

Assumption:

Div
$$\left(\rho \overrightarrow{v} \overrightarrow{u_{j}\theta'}\right)$$
 - Diff $\left(\rho \overrightarrow{u_{j}\theta'}\right) = a_{1} \frac{\overrightarrow{u_{j}\theta'}}{k} (P-\epsilon) + a_{2} \frac{\overrightarrow{u_{j}\theta'}}{\theta^{2}} (P_{\theta} - \epsilon_{\theta})$ (50)

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where:

$$P_{\theta} = -2 \overline{v_j \theta'} \frac{\partial \overline{\theta}}{\partial x_j}$$
 (51)

$$\epsilon_{\theta} = \alpha_{\theta} \frac{\epsilon}{k} \frac{\theta^{1/2}}{\theta^{1/2}}$$
 (52)

 a_1 and a_2 are empirical constants to be determined.

The transport equation for scalar fluctuations, $\theta^{\frac{1}{2}}$, is

$$\frac{\text{div }(\rho \overline{\vee} \theta^{\frac{1}{2}})}{\text{Convection}} = \underbrace{\rho \rho_{\theta} - \rho \epsilon_{\theta}}_{\text{Diffusion}}$$
(53)

where,

$$P_{\theta} = -2 \overline{u_{j}\theta'} \frac{\partial \overline{\theta}}{\partial x_{j}} = -2 \overline{u\theta'} \frac{\partial \overline{\theta}}{\partial x} - 2 \overline{v\theta'} \frac{\partial \overline{\theta}}{\partial r}$$
 (54)

and

$$\epsilon_{\theta} = \alpha_{\theta} = \frac{\epsilon}{k} = \frac{\theta^{1/2}}{\theta^{1/2}}$$
 (55)

For minimizing computational effort, the following assumption is made in a form consistent with the model for velocity fluctuations.

Assume:

$$\operatorname{div} (\stackrel{\rho \downarrow}{\nabla} \stackrel{\rho}{\theta}) - \operatorname{Diff} (\stackrel{\rho}{\theta}) \approx C_{\theta} \stackrel{\rho \theta}{= k} (P - \epsilon)$$
 (56)

Using Equations (53) and (56)

$$\rho P_{\theta} - \rho_{\epsilon_{\theta}} = C_{\theta} \frac{\overline{\rho_{\theta}^{2}}^{2}}{k} (P_{-\epsilon})$$
 (57)

With these simplifications, the correlations for scalar quantities reduce to the form:

$$- \overline{v\theta'} = \left[\overline{uv} \frac{\partial \overline{\theta}}{\partial x} + \overline{v^2} \frac{\partial \overline{\theta}}{\partial r} \right] / \left[c_{\theta} \frac{\epsilon}{k} + a_{\theta} \left(\frac{P - \epsilon}{k} \right) \right]$$
 (58)

$$-\overline{u\theta'} = \left[\overline{u^2} \frac{\partial \overline{\theta}}{\partial x} + \overline{uv} \frac{\partial \overline{\theta}}{\partial r} + \overline{v\theta'} \frac{\partial U}{\partial r} (I - c_{2\theta})\right]$$

$$\left[a_1 \left(\frac{P - \epsilon}{k}\right) + c_{1\theta} \frac{\epsilon}{k} + (I - c_{2\theta}) \frac{\partial U}{\partial x}\right]$$
(59)

$$\overline{\theta^{12}} = -2 \left[\overline{u\theta'} \frac{\partial \overline{\theta}}{\partial x} + \overline{v\theta'} \frac{\partial \overline{\theta}}{\partial r} \right] / \left[c_{\theta} \left(\frac{P - \epsilon}{k} \right) + \alpha_{\theta} \frac{\epsilon}{k} \right]$$
(60)

The assumptions used in the derivation of the algebraic stress model are applicable for the flows that are close to local equilibrium. However, this model does not neglect any of the terms in the transport equation, and only a scaling law has been employed.

The algebraic relations shown above express the turbulent scalar transport as a function of both mean scalar gradients and mean velocity gradients and hence can predict counter-gradient scalar transport.

3.3 Gaseous Fuel Combustion Models

Successful modeling of combustors depends upon a correct description and coupling of the fluid mechanics, turbulence, heat transfer, and chemical processes involved. The rates of turbulent exchange of various species and the rates of chemical change need to be modeled. In turn, this modeling will determine the details of quantities such as energy input to the gas stream, flow patterns, temperatures, and species concentrations. Turbulence models have been developed to a reasonably satisfactory stage. The state of development of chemical models is not nearly so satisfactory and is discussed in Paragraph 3.3.1.

The turbulence/chemistry interaction model currently used by Garrett is a modified version of the eddy-breakup model; work is in progress on the development of a perturbation analysis technique. These models are described in Paragraph 3.3.2.

3.3.1 <u>Hydrocarbon Reaction Mechanisms</u>

A successful modeling of combustion systems depends on an adequate description of the reaction mechanism. For hydrocarbon oxidation, a large number of species participating simultaneously in numerous elementary kinetic steps is required to specify the reaction mechanism. These differential equations are "stiff" and require special time-consuming integration methods. For a complex 3-D problem, the computing costs would be prohibitive. Besides the large number of species equations to be solved, the elementary steps and their rate constants are not well known except for the simplest of hydrocarbons (e.g., CH,). To avoid this problem, the gas turbine combustion modeling effort has frequently been simplified by using a global approach that reduces chemistry to the specification of an overall global oxidation scheme. This can predict quantities of interest: fuel consumption and heat release rates.

One Step Scheme

The simplest global mechanism is the one-step scheme:

$$C_X H_y + (X + \frac{y}{4})O_2 - XCO_2 + \frac{y}{2} H_2O$$

The advantage of this mechanism is its simplicity; it involves the solution of the conservation equations for unburned fuel and the mixture fraction. The heat release and the concentrations of the other species are then obtained from linear functions of the amount of fuel consumed. This mechanism, however, fails to predict the important characteristics of hydrocarbon oxidation, i.e., the formation of intermediates and CO, which influence the process considerably. As a result, this mechanism is inadequate for obtaining quantitative predictions.

Two-Step Scheme

A slightly more complex scheme is the two-step mechanism:

$$C_XH_Y + (\frac{X}{2} + \frac{Y}{4}) (O_2 + nN_2) \longrightarrow XCO + \frac{Y}{2} H_2O + (\frac{Y}{2} + \frac{Y}{4}) nN_2$$

 $XCO + \frac{X}{2} (O_2 + nN_2) \longrightarrow XCO_2 + \frac{X}{2} nN_2.$

This scheme involves the solution of one additional equation: that for the concentration of CO. Although the two-step scheme has been widely used by Garrett, it is deficient in that the formation of intermediates is ignored. The derivation of the pertinent equations is given below.

For the first reaction,

$$r_1 = (mass of O_2)/(mass of fuel),$$

$$r_2 = (mass of CO)/(mass of fuel),$$

$$r_3 = (mass of H_2O)/(mass of fuel);$$
(61)

in the second reaction:

$$r_4 = (mass of O_2)/(mass of CO),$$

$$r_5 = (mass of CO_2)/(mass of CO).$$
(62)

The values of these ratios can be calculated in a straight-forward manner:

$$r_{1} = (\frac{X}{2} + \frac{Y}{4}) W_{O2}/W_{fu}$$

$$r_{2} = X W_{CO}/W_{fu}$$

$$r_{3} = (Y/2)W_{H2O}/W_{fu}$$

$$r_{4} = (1/2)W_{O2}/W_{CO}$$

$$r_{5} = W_{CO2}/W_{CO}$$
(63)

Here the W's are the molecular weights of the chemical species.

The mass fractions of all chemical species obey the general differential equation with S_ϕ as defined in Table 2. Further, the diffusion coefficient Γ_ϕ can be taken to be the same for all species, especially when the flow is turbulent. The value of Γ_ϕ is then $\mu_{\rm t}/\sigma_{\rm t}$, where $\sigma_{\rm t}$ is the turbulent Prandtl (or Schmidt) number. The source terms for various species are related via the ratios defined in Equations (61) and (62). As a result, the mass fractions of the species can be added in certain proportions to yield

zero source terms. This is shown in Table 2. Here S_{fu} denotes the source for fuel due to the first reaction, while S_{CO} stands for the rate of production of CO in the second reaction.

TABLE 2. SOURCE TERMS FOR CHEMICAL SPECIES.

				_
	φ		s	
	^M fu		s _{fu}	
	m _{CO}		s _{CO} - r ₂ s _{fu}	
	^m ox		r ₁ s _{fu} + r ₄ s _{CO}	
	M _{CO2}		- r ₅ s _{co}	
	M _{H2} O		- r ₃ s _{fu}	
$\phi_{A} \equiv m_{OX} -$	$(r_1 + r_2 r_4)^m f$	iu - r ₄ m _{CO}		
$\phi_{\rm B} \equiv {\rm m_{CO}}_2$	+ r ₅ m _{CO} + r ₂ r ₅	^m fu	o	
$\phi_{\rm C} \equiv m_{\rm H_{2O}} +$	r ₃ m _{fu}		0 • • • • • • • • • • • • • • • • • • •	

The last three entries in Table 2 show that, because their source term is zero, a single solution for them would suffice provided their boundary conditions are the same. This condition can be ensured by normalizing the ϕ 's with reference to their values in the air and fuel streams. Thus a single variable f with a zero source term and with values 0 and 1 in the air and fuel streams

respectively can be regarded as providing the solutions for $\phi_{\rm A}$, $\phi_{\rm B}$ and $\phi_{\rm C}$ via the following relationships:

$$f = \frac{\phi_{A} - \phi_{A, air}}{\phi_{A, fuel} - \phi_{A, Air}} = \frac{\phi_{B} - \phi_{B, air}}{\phi_{B, fuel} - \phi_{B, air}} = \frac{\phi_{C} - \phi_{C, air}}{\phi_{C, fuel} - \phi_{C, air}}$$
(64)

Further, let:

and

$$(m_{OX})_{air} = R$$

$$(m_{N2})_{air} = 1-R$$
(65)

Combining Equations (64), (65), and the definitions of $\phi_{\rm A}$, $\phi_{\rm B}$, $\phi_{\rm C}$, we have:

$$m_{OX} = R(1-f) + r_4 m_{CO} + (r_1+r_2r_4) (m_{fu}-f)$$
 (66)

$$m_{CO_2} = r_2 r_5 (f - m_{fu}) - r_5 m_{CO}$$
 (67)

$$m_{H_2O} = r_3(f-m_{fu})$$
 (68)

Incidentally, f can be considered as the mass fraction of "total fuel" that would prevail if the fuel did not react at all.

The reaction rates S_{fu} and S_{CO} are given by the following relations:

$$S_{fu} = -$$
 (The smaller of S_1 and S_2),

where

$$S_1 = F_1^{\rho_1 \cdot 5} m_{fu}^{0.5} m_{OX} \exp(-E_1/RT),$$

 $S_2 = C_{R,1}^{\rho_1 \cdot \delta} \rho_{fu}^{\rho_2 \cdot \delta} \epsilon/k.$ (69)

Here, $C_{R,1}$ is the eddy breakup constant for first reaction. Recommended value for $C_{R,1}$ is 3.0

$$S_{CO} = -$$
 (The smaller of S_3 and S_4),

where

$$S_3 = F_2 \rho^2 m_{CO} m_{OX} \exp(-E_2/RT),$$

$$S_4 = C_{R,2} \rho^{m_{CO}} \epsilon/k.$$
(70)

 $\rm ^{C}_{R,2}$ is the eddy breakup constant for the second reation, recommended value for $\rm ^{C}_{R,2}$ is 4.0

The constants in the above expressions are given the following values:

$$F_1 = 3.3 \times 10^{14}$$
, $E_1/R = 27000$., $C_{R,1} = 3$, $E_2/R = 12500$., $E_{R,2} = 4$, all in S.I. Units.

To summarize, the quantities m_{fu} , m_{CO} , and f are used as the dependent variables of the differential equations. The source terms for m_{fu} and m_{CO} are calculated from Equation (69) and (70), while the source for f is zero. The values of m_{OX} , m_{CO_2} , and m_{H_2O} are then obtained from Equations (66), (67), and (68). Lastly, m_{N_2} is calculated from the fact that all mass fractions should add up to unity.

Four-Step Scheme

The oxidation of hydrocarbon fuel can be described by the following steps:

- (a) Transformation of the hydrocarbon fuel into intermediate hydrocarbons and hydrogen with little release of energy
- (b) Oxidation of intermediates to CO and ${
 m H_2}$
- (c) Oxidation of CO to CO2
- (d) Oxidation of H_2 to H_2O .

Steps (b) through (d) are exothermic and are responsible for the release of energy and associated temperature rise. A reaction scheme, which is designed to correctly model the oxidation process, must include a description of these steps.

The simplest mechanism that accounts for the essential features of the hydrocarbon oxidation is the following four-step scheme proposed by Hautman, et al. 19

$$C_N H_{2N+2} \rightarrow \frac{N}{2} C_2 H_4 + H_2$$
 $C_2 H_4 + O_2 \rightarrow 2CO + 2H_2$
 $CO + 1/2 O_2 \rightarrow CO_2$
 $H_2 + 1/2 O_2 \rightarrow H_2O$

which is valid only for aliphatic hydrocarbons (of the type $C_{N}^{\ H}_{2N+2}$). To accommodate a general hydrocarbon $C_{X}^{\ H}_{Y}^{\ r}$, the first two steps have been modified:

$$C_{X}H_{y} \rightarrow C_{X}H_{y-2} + H_{2}$$
 $C_{X}H_{y-2} + \frac{X}{2}O_{2} \rightarrow XCO + \frac{y-2}{2}H_{2}$

This scheme involves the solution of two transport equations for the concentrations of $C_{X}H_{Y-2}$ and H_{2} , in addition to the transport operations for unburned fuel, CO, and "total fuel" as outlined in the two-step scheme.

3.3.2 Turbulence/Chemistry Interaction

In this section, a review of turbulent combustion models is provided. This is followed by a description of the models under investigation at Garrett. Finally, a summary of turbulence/chemistry interaction modeling is provided.

Review of Turbulent Combustion Models

An adequate treatment of turbulence/chemistry interactions is essential for a reliable combustion model. Since the kinetic equations are nonlinear in temperature and concentrations, large errors can be caused by incorrect time-averaging of the various terms with attendant effects on heat release rates, time-averaged gas temperatures, and convective and radiative fluxes to the liner walls.

<u>The Problem</u> - It has long been realized that the practice of writing chemical kinetic equations in terms of time-averaged local variables such as

$$\overline{W}_{i} = \overline{Y}_{i} \overline{Y}_{j} \overline{A} \exp \left\{-\theta/\overline{1}\right\}$$
(71)

is unsound in turbulent mixing flows with relatively fast kinetics. Here W_i is the chemical reaction rate for species i of mole fraction Y_i ; Y_j is the mole fraction of another species; A is the preexponential factor in the Arrhenius expression for the chemical kinetic rate; θ is the activation temperature; and Y_i the absolute temperature, the overbar indicating time averaging. Equation (71) neglects the correlations between fluctuations in the various quantities, e.g., $\overline{Y_i^iY_j^i}$, $\overline{Y_i^iT_i^i}$ and the contributions from these terms can change the computed reaction rate by an order of magnitude or more. Attempts to compute the various correlations directly, as has been done by Donaldson Y_i^{i} and Borghi, Y_i^{i} have proved successful only in flows where the fluctuations are low and the heat release is not large.

The Fast-Chemistry Approach - A more satisfactory approach in non-premixed combustion systems is based on the assumption that the chemistry is fast. The chemical reaction rates are then entirely mixing controlled and are a function of the turbulence rather than the chemical kinetics. Two versions of this approach are in current use.

In the first version, equations for conserved scalars such as the element mass fractions or the mixture fraction are solved, instead of solving directly for the individual combustion product species. Molecular species concentrations and temperature are then determined from the computed moments of the conserved scalar, usually by assuming some probability density function for the conserved scalar. The fast chemistry assumption implies an instantaneous relationship between molecular species or temperature and the conserved scalar. Chemical reaction rates can be found, if needed, by differentiation. Such an approach has been used by some investigators, e.g., Lockwood. The problem is that the extension to include the treatment of any type of feaction mechanism, even a single-step one, entails complications.

In the second version, molecular equations are solved and the chemical reaction rate is modeled directly in terms of turbulence quantities. The Spalding eddy breakup (EBU) model²³ is the prime example of this approach, in which single or multi-step reaction mechanisms can be handled, when suitable modifications to the model are made. This has been done by Garrett, which has developed a modified version of this model.

Both of these approaches give qualitatively satisfactory results for the main species concentrations and temperature. The problem, however, is that chemical kinetics is no longer involved.

The Inclusion of Chemical Kinetics - Although the majority of fuel oxidation in gas turbine combustion systems is essentially mixing controlled under most operating conditions, the chemical kinetic effects must be included to predict hydrocarbon emissions, flame stabilization or blowout, CO emissions, soot formation and burnout, and NO formation. The problems of satisfactorily including the chemical kinetics into the chemical reaction rate have proved to be formidable.

As a first step towards inclusion of the kinetics, the EBU model has been modified at Garrett to compute the reaction rate R from the minimum of the EBU rate and the well-stirred reactor global reaction rates. Garrett has used 2-step and, recently, 4-step kinetic schemes. The procedure is illustrated here with a single-step reaction scheme.

$$R = \min [R_{EBU}, R_{WS}]$$
 (72)

$$R_{EBU} = C_{R} \rho \phi \epsilon / k \tag{73}$$

$$R_{WS} = A \rho^{1.5} M_{ox} M_{fu}^{0.5} \exp(-E/RT)$$
 (74)

$$\phi = \min \left[M_{fu}, M_{Ox} / i \right] \tag{75}$$

where:

R_{ERII} = the eddy-breakup rate of chemical reaction;

 R_{WS} = the well-stirred rate of chemical reaction;

C_p = empirical constant;

A = Arrhenius pre-exponential factor;

 ρ = density;

 M_{OX} = mass fraction of oxidant

 M_{fin} = mass fraction of fuel

E/R = activation temperature;

T = absolute temperature;

k = turbulence kinetic energy

 ϵ = dissipation rate of k

i = mass of oxidant per unit mass of fuel.

This model, which was used in the computer codes developed by Garrett for the US Army, 12 has been found suitable for qualitative correlations. A further extension of the model at Garrett solves a transport equation for the fluctuation, $g = (-\phi^2)$, of the fuel concentration rather than obtaining ϕ from Equation (75). This additional equation results in better agreement between the predictions and experimental data for typical combustor geometries. It is still not suitable for accurate quantitative predictions and for problems such as kinetic effects on temperature or satisfactory

estimates of free-radical concentrations. These quantities are required for accurate prediction of CO, since CO consumption often occurs via the reaction $CO + OH = CO_2 + H$.

Achievement of a satisfactory approach to the modeling of the chemical reactions has led to several rather novel approaches to the problem. Many of these methods, such as Spalding's ESCIMO model, 24 Chorin's Vortex Dynamics, large eddy simulation techniques, and joint PDF approaches, 25 involve at least an order of magnitude increase in the size and complexity of the computation and as yet are not completely formulated. One approach, based on a perturbation analysis for reaction kinetics, does not involve such an increase in size and complexity, and has been formulated by Bilger. 26 This method, as described in the next paragraph, has been adapted by Garrett.

The Perturbation Analysis for Reaction Kinetics

In this approach, a turbulent diffusion flame model has been developed. 27 It uses a double reaction zone model and perturbation analysis for finite rate kinetics for hydrocarbon combustion. system of eight parabolic transport equations is solved. The system consists of the usual $k-\epsilon$ model equation in Favre averaged form for continuity, momentum, mean mixture fraction, specific turbulent kinetic energy, and turbulent kinetic energy dissipation rate, with additional scalar transport equations for mixture mole number pertubation, unburned fuel mass fraction pertubation, and mixture The thermodynamic state (and composition) of fraction variance. the flow field is contained in an equilibrium model of the hydrocarbon-air mixture in terms of mean mixture fraction. The progress of the chemical reactions (and thereby the molecular kinetic rates) is contained in perturbations or constraints on the equilibrium in terms of mole number and unburned fuel mass fraction. The unburned

fuel mass fraction and the intermediate are specified as functions of mixture mass fraction, ξ . For the fuel,

$$Y_{13} = Y^{\circ}_{13} + y$$
 (76)

where

$$Y^{\circ}_{13} = 0 \qquad 0 \le \xi < \xi \text{ig}$$

and

$$Y^{o}_{13} = \frac{(\xi - \xi_{ig})}{1 - \xi_{ig}}$$
 $\dot{\xi}_{ig} < \xi \le 1$

where

y is the pertubation in fuel mass fraction

Y°₁₃ is the "fast chemistry" (i.e., zero pertubation) fuel mass fraction

 Y_{13} is the fuel mass fraction

is the mixture fraction where a "reaction sheet" consumption or pyrolysis of fuel occurs under fast chemistry conditions similar to the classical Burke-Schumann formulation. ξ_{ig} here is taken as 0.073.

For the intermediate hydrocarbon, its mass fraction is given by,

$$Y_{12} = 0 \qquad 0 \le \xi \le \xi_s \tag{77}$$

$$Y_{12} = \frac{e\Gamma}{1 - \xi_s} \qquad (\xi - \xi_s) \qquad \xi_s < \xi \le \xi_{ig}$$
 (78)

$$Y_{12} = \frac{e\Gamma(\xi_{ig} - \xi_s)}{(1 - \xi_s)(1 - \xi_{ig})}$$
 $(1 - \xi)$ $\xi_{ig} < \xi \le 1$ (79)

where

 Γ is the mass fraction of fuel in the inlet fuel stream

Y₁₂ is the intermediate hydrocarbon mass fraction

e is the fraction of fuel by mass that is converted to intermediate at ξ_{ig} for fast chemistry conditions. e is taken as 0.2

and ξ_s is the stoichiometric mixture fraction

Hence, the double reaction zone at ξ_{s} and ξ_{iq} .

Thirteen species are considered in the reactions. H, $\rm H_2$, $\rm H_2O$, O, OH, O₂, $\rm HO_2$, $\rm N_2$, Ar, CO, and CO₂ are calculated from partial or constrained equilibrium, and the fuel and intermediate are specified as in Equations 76-79. The pertubation in mole number space is a result of the rate of three-body recombination reactions,

$$H+H+M \longrightarrow H_2 + M$$
 R1

$$H+OH+M \longrightarrow H_2O + M$$
 R2

$$H+O_2+M \longrightarrow HO_2 + M$$
 R3

$$H+O+M \longrightarrow OH + M$$
 R4

The progress of these reactions toward equilibrium is measured by mole number, $\ensuremath{\mathtt{N}}$

$$N = \sum_{i=1}^{11} \frac{Y_i}{W_i} \frac{Mole}{Kg}$$
 (80)

where

Y; is the mass fraction of species i

and

 W_{i} is the molecular weight of species i

The pertubation in mole number is defined as

$$n = N - N^0 \tag{81}$$

Where N° is the number of moles at full equilibrium. Then, for various pertubations in mole number space for a given mixture mass fraction, the time rate of change of N can be calculated from reactions R1-R4 using here the kinetic data of Jensen and Jones.²⁸

Perturbation Equations

From the species balance transport equation,

$$\frac{\partial Y_{i}}{\partial t} + \rho U_{k} \frac{\partial Y_{i}}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \left(\rho^{D} \frac{\partial Y_{i}}{\partial x_{k}} \right) = 0$$
 (82)

where the molecular diffusivity is assumed to be the same for all species, and using Equations 80 and 81 gives,

$$\frac{\partial n}{\partial t} + \rho \cup_{k} \frac{\partial n}{\partial x_{k}} + \frac{\partial}{\partial x_{k}} \left(\rho D \frac{\partial n}{\partial x_{k}} \right) = \rho D \left(\frac{\partial \xi}{\partial x_{k}} \right)^{2} \frac{d^{2} N^{\rho}}{d \xi^{2}} + w_{n}$$
 (83)

 $\mathbf{w}_{\mathbf{n}}$ is the source term for mole number

A similar equation can be written for the fuel mass fraction perturbation.

$$\frac{\partial y}{\partial t} + \rho \cup_{k} \frac{\partial y}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \left(\rho D \frac{\partial y}{\partial x_{k}} \right) = \rho D \left(\frac{\partial \xi}{\partial x_{k}} \right)^{2} \frac{d^{2}Y^{o}_{13}}{d\xi^{2}} + w_{y} \quad (84)$$

 $\mathbf{W}_{\mathbf{y}}$ is the source term for mass fraction where the dependence of \mathbf{y} on \mathbf{N}° is neglected.

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Then using density weighting (Favre averaging), the equations for turbulent flow become,

$$\overline{\rho} \quad \widetilde{v}_{\mathbf{k}} \quad \frac{\partial \widetilde{\mathbf{n}}}{\partial x_{\mathbf{k}}} + \frac{\partial}{\partial x_{\mathbf{k}}} \left(\overline{\rho} \quad \widetilde{\mathbf{v}}^{"} \widetilde{\mathbf{n}}^{"} \right) = \rho D \left(\frac{\partial \xi}{\partial x_{\mathbf{k}}} \right)^{2} \quad \frac{d^{2} N^{o}}{d \xi^{2}} + \overline{w}_{\mathbf{n}}$$
 (85)

$$\overline{\rho} \quad \widetilde{v}_{k} \quad \frac{\partial \widetilde{y}}{\partial x_{k}} + \frac{\partial}{\partial x_{k}} \left(\overline{\rho} \quad \widetilde{v}'' \widetilde{y}'' \right) = \rho D \left(\frac{\partial \xi}{\partial x_{k}} \right)^{2} \quad \frac{d^{2} Y^{o}}{d \xi^{2}} |3| + \overline{w}_{y}$$
 (86)

Using gradient modeling of the turbulent fluxes and $k-\epsilon$ modeling of the scalar dissipation X

where

$$X = 2 D \left(\frac{3 \xi^{11}}{3 x_{k}} \right)^{2}$$
 (87)

the Favre averaged scalar dissipation rate is

$$\chi = C_{g_2} \epsilon^{\kappa 2} (\epsilon/k)$$
 (88)

where C_{g_2} is a model constant with value of 1.79. Then,

$$\overline{\rho} \widetilde{v}_{k} \frac{\partial \widetilde{n}}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \left[\frac{\mu_{eff}}{\sigma_{n}} \frac{\partial \widetilde{n}}{\partial x_{k}} \right] = 1/2 \overline{\rho} C_{g_{2}} \widetilde{\xi^{"2}} \left(\epsilon/k \right) \Delta_{N, s} \widetilde{p} \left(\xi_{s} \right)_{(89)} + \overline{w}_{n}$$

$$\overline{P} \widetilde{v}_{k} \frac{\partial \widetilde{y}}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \left[\frac{\mu_{\text{eff}}}{\sigma_{y}} \underbrace{\partial \widetilde{y}}_{\xi_{k}} \right] = 1/2 \overline{P} C_{g_{2}} \widetilde{\xi_{\parallel}^{2}}^{2} (\epsilon/k) \Delta_{y} \widetilde{P}(\xi_{ig}) (90) + \overline{w}_{y}$$

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The parameters $\Delta_{N,s}$ and Δ_{y} represent the net change in $dN^{\circ}/d\xi$ and $dY^{\circ}_{13}/d\xi$ across the reaction zones at ξ_{s} and ξ_{ig} , respectively, and $p(\xi)$ is the Favre probability density of ξ . In deriving these equations, the usual high Reynolds number assumptions have been made and the scalar dissipation is assumed not to be correlated with the mixture fraction.

Finally, the mixture fraction pertubation,

gives the transport equation for the variance of the mixture fraction

$$\overline{\rho} \ \widetilde{\upsilon}_{k} \ \frac{\partial \xi^{\widetilde{n}^{2}}}{\partial x_{k}} - \frac{\partial}{\partial x_{k}} \left(\frac{\mu_{eff}}{\sigma_{\xi^{\widetilde{n}^{2}}}} - \frac{\partial \xi^{\widetilde{n}^{2}}}{\partial x_{k}} \right) = C_{g_{1}} \mu_{eff} \left(\frac{\partial \xi^{\widetilde{n}^{2}}}{\partial x_{k}} \right)^{2} - C_{g_{2}} \overline{\rho} \epsilon^{\frac{\widetilde{\xi}^{\widetilde{n}^{2}}}{r}}$$
(91)

The main features of measured probability density functions are the strong spike associated with the free stream and the continuous distribution generated by turbulence. By splitting the two, a clipped Gaussian intermittent formula is used to represent the Favre averaged probability density at a particular value, ξ_{γ}

$$\widetilde{p}\left(\xi_{\alpha}\right) = \frac{\gamma}{\sqrt{2\pi} \left(\xi^{\widetilde{n}^{2}}\right)_{t}^{1/2}} \quad \exp \quad \left\{ -\frac{1/2}{2} \frac{\left(\widetilde{\xi}_{t}^{2} - \xi_{\alpha}\right)^{2}}{\left(\xi^{\widetilde{n}^{2}}\right)_{t}^{2}} \right\}$$
where
$$\widetilde{\xi}_{t}^{2} = \widetilde{\xi}/\widetilde{\gamma}$$

$$\widetilde{\gamma} = 1 \quad \text{for } \widetilde{\xi^{\widetilde{n}^{2}}} < 0.25 \ \widetilde{\xi}^{2}$$

$$\widetilde{\gamma} = \frac{1.25}{\xi^{\widetilde{n}^{2}}/\xi^{2} + 1} \quad \text{for } \widetilde{\xi^{\widetilde{n}^{2}}} \ge 0.25 \ \widetilde{\xi}^{2}$$

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and

$$\left(\widetilde{\varepsilon}^{"2}\right) = \widetilde{\gamma} \left[\left(\widetilde{\varepsilon}^{"2}\right)_{\dagger} + \left(\widetilde{\varepsilon}_{\dagger} - \widetilde{\varepsilon}\right)^{2}\right] + \left(1 - \widetilde{\gamma}\right)\widetilde{\varepsilon}^{2}$$
(93)

Also from simple fits to the partial equilibrium calculations, the mean density as a function of the mole number and fuel mass function pertubations is

$$\frac{1}{\rho} = \left[v^{\bullet}(\xi) \right]^{-1} + \widetilde{\gamma} \left(0.022 \, \widetilde{n} + 1.38 \, \widetilde{\gamma} \right)$$
(94)

where v° (ξ) is the Favre average specific volume for zero perturbations.

Lastly, the kinetic dependent source erms $\overline{w_n}$ and $\overline{w_y}$ are given by,

$$\overline{w}_{n} = \overline{\rho} \iiint q(\xi, n, y) w_{n}(\xi, n, y) (1/\rho) \widetilde{p}(\xi, n, y) d\xi dn dy$$
(95)

and
$$\overline{w}_y = -\overline{\rho} \iiint S_y^* (\xi, n, y) \widetilde{p}(\xi, n, y) dy dn d\xi$$
 (96)

where
$$w_n/\rho = -9000 n^2 \frac{\text{moles}}{\text{kg sec}}$$

from consideration of the partial equilibrium calculations and $q(\xi, n, y)$ is a quenching function to allow for breakdown of the constrained equilibrium represented as follows:

$$q(\xi, n, y) = B*(\xi) = 0 for \ \widetilde{\xi} < 0.01$$
$$= 50 (\widetilde{\xi} - 0.01) 0.01 \le \widetilde{\xi} \le 0.03$$
$$= 1 \widetilde{\xi} > 0.03$$

Simplification of the joint P.D.F. yields

$$\overline{w}_{n} = -\rho B* 9000 \tilde{n}^{2}$$

The fuel source term w_y is evaluated based on the kinetic rate of Duterque²⁹ over the range of expected values of ξ , n, and y and again the joint P.D.F. is avoided, as

$$\overline{W}_{y} = -\overline{\rho} \int_{0}^{1} S_{y}^{*}(\xi, \widetilde{n}, \widetilde{y}) \widetilde{P}(\xi) d\xi$$

$$S_{y}^{*} = \frac{W_{y}}{\rho} = 8.53.10^{14} \left(\frac{\chi_{o_{2}} Y}{T}\right) \exp\left(\frac{-23500}{T}\right) \sec^{-1}$$
(97)

where

where Xo2 oxygen mole fraction and temperature, T, are taken from the partial equilibrium calculations for Methane.

The above three differential equations are combined with the other five Favre averaged equations, as mentioned above, written in cylindrical coordinates and transformed using the stream function

$$\partial \psi = \rho \widetilde{\mathbf{u}} \mathbf{r} \partial \mathbf{r}$$

and put in finite difference form using a Crank-Nicholson central difference scheme. The nonlinear coefficient terms and source terms were evaluated as the mean of the upstream value and the first estimate of the downstream value.

Then, for any "output" position in the flame, the effect of pertubations on species mole fractions and temperature is calculated from the local P.D.F.,

$$\widetilde{X}_{i} = \int_{0}^{1} X_{i} (\xi, \widetilde{n}, \widetilde{\gamma}) \widetilde{P} (\xi) d\xi$$

$$\widetilde{T} = \int_{0}^{1} T (\xi, \widetilde{n}, \widetilde{\gamma}) \widetilde{P} (\xi) d\xi$$
(98)

again, where joint probabilities have been avoided.

3.4 Spray Evaporation/Combustion Models

Since the influence of the liquid fuel spray on combustor performance is quite pronounced, an accurate spray model is essential for any combustor modeling effort. The modeling of liquid fuel sprays is discussed in this section.

The spray model currently used by Garrett is based on a Lagrangian discrete-droplet approach allowing for droplet slip but no turbulent dispersion. Eulerian (continuous formulations) versions allowing for dispersion, with or without droplet slip, have also been developed by Garrett. Both approaches offer advantages in certain circumstances.

3.4.1 A Review of Spray Models

A number of spray evaporation/combustion models have been developed and used with varying degrees of success. Several review papers are available in the literature; 30,31 an excellent recent review paper is by Faeth. 32 Faeth has divided the spray model work into two major categories:

- o Locally homogeneous flow (LHF) models
- o Separated flow (SF) models

In LHF models, the gas and liquid phases are assumed to be in dynamic and thermodynamic equilibrium at all times, with no droplet slip. Consequently, the use of LHF models should be limited to finer droplet sprays. Although the LHF predictions tend to approach measurements as the droplet size reduces, the agreement is relatively poor, even for the sprays that have an SMD of around 30 microns. Compared to the SF models, the LHF models are easy to use because they require minimum information concerning fuel injector characteristics, fewer empirical constants, and shorter computation time. The LHF models give useful qualitative descriptions of the spray development, the rate of which is generally overestimated.

In SF models, finite interphase transport processes of mass, momentum, and heat are taken into account; and these models are therefore of more interest in gas turbine combustor modeling. The SF models can be broadly divided into the following two major categories:

- o Discrete Droplet Models (DDM) Lagrangian
- o Continuous Formulation Models (CFM) Eulerian

Both categories contain features that make their application to practical combustors desirable. In DDM, the fuel droplets are assumed to exist sufficiently removed from each other that droplet-to-droplet interaction can be neglected. This assumption is quite reasonable for regions in the combustor other than very close to the fuel nozzle spray origin. Thus, the analytical modeling of a single droplet can be applied to the gas turbine spray that greatly simplifies the formulation. The nozzle spray is divided into a number of size groups usually determined experimentally, 33 with one droplet representing the behavior of all the droplets in its group. A DDM is constructed for each size group. Given an initial velocity and temperature as determined from the injector characteristics, the droplet trajectory is calculated through the flow domain

as governed by drag and other forces, until the droplet evaporates or exits the calculation grid. At each point along the flight path as evaporation occurs, modifications are made to the momentum, enthalpy, and species equations that govern the gas phase flow.

The second major category of SF models is CFM. These models solve turbulent transport equations for the motion of the droplets and the turbulent diffusion of droplets is included. An underlying assumption is that all the droplets and the gas phase have the same velocity. The computational effort required for CFM is greatly increased because a complete equation (similar to the momentum, species, etc., equations) must be solved for each droplet group. Computer storage must also be allocated for the extra variables. A major disadvantage of this approach is that errors are generated in the vicinity of the fuel nozzle. Since the difference in the liquid and gas phase velocities is very significant in this region, a better resolution of grid spacing is needed than can be managed.

3.4.2 Garrett's Spray Models

The main requirement of a spray model is accurate predictive capability within a pasonable amount of computational effort, especially for 3-D flows of practical interest. To achieve accuracy, various physical processes must be incorporated into the model in a realistic manner. Thus, relative velocity differences between the gaseous and liquid phases (droplet slip), resulting in interphase momentum transfer, must be considered. Also, the evaporation of droplets during heat-up time (interphase heat and mass transfer) is important in order to predict ignition processes. Finally, turbulent diffusion of droplets is important but is generally ignored in most of the spray models. Stochastic models to consider turbulent diffusion, as reported by Gosman³⁵ are computationally expensive when applied to real combustors.

On the computational aspect of spray modeling, it should be realized that a different degree of resolution is required in the near-injector and far-injector regions.

Consideration of these factors has led to the development of the Garrett spray models, the features of which are described below.

Evaporation during heat-up time is considered in the Garrett model and the computation of heat-up and evaporation rates includes realistic properties of jet aviation fuels. The spray model is applicable to both dense and sparse sprays and is coupled into either the 2-step or the 4-step global hydrocarbon oxidation scheme; it is available in both 2-D and 3-D combustor performance programs.

Velocity differences (slip) between the droplets and the gas phase are modeled, and so is turbulent diffusion of the droplets. For computational purposes, the droplet size distribution is discretized, differential equations in a Eulerian framework are solved for the velocity components and concentration of droplets in each size group (typically five size groups are considered). To obtain good resolution in the near injector region, Lagrangian equations of motion for the droplets are solved in this region. Each class of droplets is tracked through the flow field in the vicinity of the injector and the interphase transports of mass, momentum, and energy are used to couple this solution to the Eulerian equations. The model thus combines the desirable features of the DDM and CFM approaches.

Lagrangian Model

The Lagrangian model was initially pursued since the formulation allows the tracking of small fuel droplets that are significantly smaller than typical grid dimensions and since the computational requirements for 3-D flows are quite small. In addition, the assumption of sparse sprays and no droplet-droplet interaction is quite reasonable for most regions in a gas turbine combustor.

The generalized governing equation for fuel mass fraction is

$$\operatorname{div}\left(\rho \overrightarrow{\mathsf{Vm}}_{\mathsf{fU}} - \mathbf{r}_{\mathsf{fU},\mathsf{eff}} \operatorname{grad} \mathbf{m}_{\mathsf{fU}}\right) = \mathring{\mathsf{m}}_{\mathsf{e}}^{\mathsf{II}} - \mathsf{R}_{\mathsf{fU}}$$
(100)

where R_{fu} is the destruction rate of fuel and $m_e^{""}$ is the rate of vapor production from the fuel droplets. The vapor production rate or evaporation rate is determined from the burning rate constant k_O , which relates the change in the square of the droplet diameter (D) with time.

$$k_o - \frac{d(-D^2)}{dt} = \frac{8\lambda_I}{\rho_f C_{PI}} \ln(I + B)$$
 (101)

where:

 λ_1 = Thermal conductivity of vapor

 C_{Pl} = Weighted average specific heat of vapor and air

B = Mass transfer number

 $\rho_{\rm f}$ = Fuel density

From the burning rate constant, the fraction of fuel evaporated from a group of droplets (ΔF_i) can be determined from the time integral;

$$\Delta F_{i} = \frac{1.5}{\rho_{f} D_{i}} \int_{0}^{\infty} \rho_{f} D_{i} k_{i} dt \qquad (102)$$

where D_{io} is the initial droplet diameter and the i subscript denotes parameters of the ith droplet group.

The total evaporation rate is then given by

$$\dot{m}_{e}^{"} = \frac{\dot{m}_{fU}}{N\Delta V} \sum_{i=1}^{N} \Delta F_{i}$$
 (103)

where:

 $\dot{\mathbf{m}}_{\mathbf{f}\mathbf{u}}$ = The total fuel flow rate

N = Number of droplet groups

ΔV = Volume of grid cell through which droplet is passing

The calculation of $\mathring{\mathbf{m}}_{e}^{"}$ given above is based on the model of Williams, 30 which uses the temperature difference between the droplet and ambient as the driving force. An alternate approach is that of Priem and Heidmann, 36 who use the partial pressure of the fuel vapor as the driving force. The advantage of the Priem and Heidmann technique is its applicability to low temperature situations such as altitude ignition, unlike the Williams model.

The expression for evaporation rate for the Priem and Heidmann model

$$\mathring{\mathbf{m}}_{\mathbf{e}}^{\mathbf{m}} = \pi D^2 \, \mathbf{K} \, \mathbf{P}_{\mathbf{vap}} \, \alpha \tag{104}$$

where:

K = Function of vapor diffusivity and droplet Reynolds number P_{vap} = Vapor pressure of fuel at droplet surface

$$\alpha = \frac{P_{\infty}}{P_{\text{vap}}} \text{ In } \left[\frac{P_{\infty}}{P_{\infty} - P_{\text{vap}}} \right]$$

 P_{∞} = Ambient pressure

Eulerian Model

The salient features of the model are (a) velocity differences (slip) between the droplets and gas phase are allowed; and (b) turbulent diffusion of the droplets is included. For computational purposes, the droplets are considered to be present in a certain number (typically 5 to 10) of discrete size ranges. Differential equations in an Eulerian framework are solved for the velocity components and concentrations of the droplets in each size group. terphase transport of mass and energy (due to droplet evaporation and combustion) and momentum (due to drag between gas and liquid phases) are taken into account. Turbulent diffusion of drops is treated as if the droplets were present as a gaseous constituent. The approach used here is to assume the diffusion to be governed by a Fickian type law with an appropriate turbulent Schmidt number, assumed to be uniform over the flow field; but this is easily extended by specifying the turbulent Schmidt number as a function of local flow characteristics. The model is applicable to both dense and sparse sprays insofar as the volume occupied by the droplets is included in the governing equations.

The partial differential equations governing the droplet motion and concentration of each size group are all written in one general form as

$$\frac{\partial}{\partial t} (R\rho\phi) + \text{div} \left\{ R \left(\overline{\rho u}\phi - \frac{\mu}{\sigma \phi} \operatorname{grad} \phi \right) \right\} = S_{\phi}$$
 (105)

where: R = Volume fraction of the droplet size considered

 ρ = Density of the droplets

 ϕ = Velocity component or concentration of droplet size considered

U = Velocity vector of aroplet size considered

 μ = Turbulent viscosity

 σ_{d} = Effective Schmidt number

 S_{ϕ} = Source of ϕ .

The term S_{ϕ} contains the pressure gradient, surface friction, and interphase drag if ϕ is a velocity component; interphase mass transfer (evaporation rate) if ϕ is droplet concentration; and interphase heat transfer (heat-up) if ϕ is the enthalphy.

A drawback of the Eulerian model is that it cannot give adequate resolution in the near injector region. An excessively fine finite-difference grid would be required to obtain adequate resolution. The Lagrangian method is capable of providing this resolution in the near injector region. Garrett has therefore coupled two methods in order to utilize the advantages of each. The method is described next.

Lagrangian/Eulerian Model

The concept of this model is analogous to the near-wall treatment described in Paragraph 3.2 and it can be called the near-noz-zle spray treatment. The interaction between the Lagrangian and Eulerian solution is through the boundary conditions and the source terms.

To obtain good resolution in the near-injector region, a special treatment is used in this region. The gas properties evaluated by the Eulerian solution are used to solve a set of Lagrangian equations of motion for the droplets again allowing for

interphase mass, momentum, and energy transfer. Each class of droplets is tracked through the flow field in the vicinity of the injector and the interphase mass, momentum, and energy transport that appear as source terms in the gas phase equations are thus evaluated. These terms are obtained by summing overall droplet size groups for each elementary control volume. The Eulerian equations are then solved again including the interphase transport items. The procedure is repeated until it converges to the desired degree of accuracy.

Physical Processes

The physical processes involved in spray modeling are interphase momentum transfer (drag forces), interphase heat transfer (droplet heat-up) and interphase mass transfer (droplet evaporation), and turbulent dispersion of droplets. A brief description is provided in the following paragraphs.

<u>Drag Forces</u> - To calculate the drag forces on the droplet, the drag coefficient, C_D , must be determined. Several expressions are available and Garrett has adopted the suggestion of Briffa³⁷ who measured water droplet velocity decay using a shadowgraph technique. Other forces, such as buoyancy or gravity, acting on the droplet, are quite small in comparison to drag and are usually neglected.

Droplet Heat-Up and Evaporation - Calculation procedures for the rate of phase change of droplets fall into two basic categories: two-stage and transient heat-up models. In two-stage models, as discussed by Williams, 30 the droplet is assumed to heat up to the boiling temperature with no evaporation occurring. Once obtained, the evaporation rate is governed by expression for the burning rate constant, defined as the time rate of change of the square of the

droplet diameter. Expressions can be used that account for the existence of an envelope or wake-type flame. The driving force is the temperature difference between the droplet and the surrounding gas phase.

Transient heat-up models such as that of Priem and Heidmann, ³⁶ use the difference in fuel vapor concentrations between the droplet surface and its surroundings as the driving force. The temperature of the drop is determined from the consideration of heat transfer to the drop and the fuel latent heat of vaporization.

Though it offers the advantage of ease of computation, the two-stage models best represent droplets in the high-temperature zones of the combustor, where droplet heat-up time is quite short and local fuel concentration is low.

Droplets exist for a significant period of time in the relatively cool, fuel-rich zone near the nozzle. The transient models better represent such droplets. The transient models are more complex from a computation standpoint, but they reflect the varying boiling temperature through the droplet life history and are superior in predicting the evaporation in low-temperature environments (during an altitude start, for example).

To evaluate the evaporation rates, fuel properties such as specific heat and distillation curves are required. For typical aviation fuels, these properties are usually available in the literature or can be estimated from basic characteristics such as specific gravity. 38

<u>Turbulent Diffusion of Droplets</u> - In most of the spray models, turbulent dispersion of droplets is ignored or introduced in an oversimplified manner. Some recent studies have adopted a stochastic approach to model this feature. Recently, Gosman, et al., 35 have

presented a stochastic discrete droplet method. In this method, a statistically significant number of random droplet samples is tracked in a Lagrangian framework and the ensemble-averaged behavior is assumed to represent the turbulent dispersion of droplets. This procedure is likely to be computationally expensive for real combustors where a large number of samples is required to obtain statistical averages.

The Garrett Eulerian model includes turbulent diffusion. The model of diffusion of droplets is assumed to be the same as that of the gaseous phase; the extent of diffusion is controlled through the specification of the turbulent Schmidt number for droplet diffusion.

3.5 Soot Formation and Oxidation

In this paragraph, soot formation and oxidation in combustion chambers are discussed. A general background on soot emissions is provided first. Quasi-global expressions for soot formation and oxidation are described. A description of the influence of turbulence on soot formation and oxidation is included. The current approach adopted by Garrett is described next. This approach considers the influence of turbulent fluctuations on soot formation and oxidation rates.

3.5.1 Background

The particulate emission of primary concern in the combustion of hydrocarbon fuels is soot, which is evident in the form of exhaust smoke. The emission of smoke from gas turbine engines is responsible for the following problems of concern in this program:

- O Higher liner temperatures due to increased radiative heat transfer
- o Impingement of carbon on metal surfaces, resulting in erosion and reduced equipment lifetimes
- o Distortion of fuel spray distribution due to carbon deposits, leading to hot spots.

Recently, attention is being directed toward the combustion of alternate fuels derived from coal liquids and shale oil. Since the use of these fuels results in significant increases in smoke production, a better understanding of the physical and chemical processes governing soot production is needed.

The processes governing the formation and subsequent oxidation of soot are of a particularly complex nature and, as such, quantitative models of soot production have yet to be developed. Soot is not an equilibrium product of combustion and, therefore, its formation is influenced as much by the physical processes of atomization, evaporation, and fuel/air mixing as by reaction kinetics. Soot is generally produced anywhere within the combustor where fuel/air mixing is inadequate, resulting in oxygen-deficient, high-temperature zones.

For the pressures and temperatures normally prevalent in gas turbine combustors, equilibrium calculations indicate that solid carbon appears when there is insufficient oxygen to oxidize the hydrocarbon to CO and H₂ according to the relation:

$$C_{x}H_{y} + \frac{x}{2}O_{2} \rightarrow xCO + \frac{y}{2}H_{2}$$
 (106)

That is, the carbon-oxygen mass ratio for incipient soot formation is 12:16, or alternatively, the atomic C-O ratio is unity. However, since soot formation is essentially a nonequilibrium phenomenon, experimentally, soot is observed at C-O ratios (a) much less than unity at low temperatures (<2000°K); and (b) greater than unity at higher temperatures.³⁹

Smoke levels are primarily dependent on

- o Air/fuel mixing
- o Temperature
- o Equivalence ratio
- o Residence time of air/fuel mixture
- o Pressure
- o Fuel composition.

These factors influence both the formation and subsequent oxidation of soot and are dependent on engine operating conditions, details of the combustor internal flow field, fuel droplet characteristics, etc.

3.5.2 Quasi-Global Models of Soot Formation and Oxidation

Since the elementary steps in the formation and oxidation of soot are not totally understood, Garrett uses quasi-global models that characterize soot production occurring via a few overall steps. Such models have been successful in predicting soot production. 40

The quasi-global models do not predict the size of soot particles. With the current state-of-the-art, it is not possible to predict the size of formation of the soot particles in any practical flow situation. Therefore, it is assumed that particles are produced at a known size in any analysis. It may also be assumed that particles are produced in accordance with a specified size distribution (e.g., Gaussian).

Tesner, et al., 41 proposed a soot production model that grouped the complex processes of pyrolysis, nuclei formation, and soot formation into three rate-limited subglobal steps:

Pyrolysis:

$$n_0 = a_0 C_{fu} \exp(-E/RT) (part./m^2.s)$$
 (107)

Nuclei Formation:

$$R_{n,f} = n_0 + (f-g)n - g_0 Nn(part_0/m^3.s)$$
 (108)

Soot Formation:

$$R_{s,f} = m_p (a - bN)n (kg/m^3.s)$$
 (109)

where a_0 , E, g, g_0 , a, and b are constants for given fuel; n_0 is the rate of spontaneous formation of nuclei; n is the nucleus concentration; N is the concentration of soot particles; and m_p is the mass of a soot particle.

Khan and Greeves 42 proposed a single-step global expression as a function of the partial pressure of unburned hydrocarbons ($^{\rm P}_{\rm HC}$), the unburned equivalence ratio ($^{\phi}_{\rm HC}$), and the temperature (T):

$$\frac{dC_s}{dt} = 0.468P_{HC}\phi_0^3 \exp(-40,000/RT) \text{ gm/cm}^3 s.$$
 (110)

In both the above models, soot oxidation rates are not considered.

Edelman, et al, 40 consider both soot formation (R_f) and soot oxidation (R_{Ox}) and express the net soot formation rate as

$$\frac{dC_s}{dt} = R_f - A_f R_{ox}$$
 (111)

where A_t equals total surface area available for oxidation. The formation step is expressed by a modified Arrhenius type of relation:

$$R_{f} = AT^{\alpha}C_{HC}^{\alpha}C_{O_{2}}^{b} \exp(-E/RT) \text{ gm/cm}^{3}s.$$
 (112)

where CO_2 , C_{HC} equal the concentration of unburned oxygen and hydrocarbon (gm/cm³), and where A, α , a, b, E are model constants.

For the oxidation step, Edelman, et al., 40 adopt the semi-empirical formula of Nagle and Strickland-Constable 43 for pyrolytic graphite oxidation; this formula is nonlinear and non-Arrhenius in PO2 and T:

$$A_{t}R_{ox} = 12 \left[\left(\frac{K_{A}P_{O_{2}}}{I+K_{Z}P_{O_{2}}} \right) \psi + K_{B}P_{O_{2}}(I-\psi) \right] A_{t}gm/s$$
(113)

where:

$$\psi = [I + K_T/(K_B P_{O_2})]^{-1}$$
 (114)

$$K_{\Delta} = 20 \exp(-30,000/RT)$$
 (115)

$$K_{\rm B} = 4.46 \times 10^{-3} \exp(-15,200/{\rm RT})$$
 (116)

$$K_T = 1.51 \times 10^5 \exp(-97,000/RT)$$
 (117)

$$K_Z = 21.3 \exp(4100/RT)$$
 (118)

Shock-tube measurements 44 of soot oxidation rates qualitatively confirm the features of the above formula. With these expressions for soot formation and oxidation and assuming a single soot particle size of 250Å, Edelman, et al., 40 obtained close agreement of the predicted soot concentration (mg/l) with the experimental data in a jet-stirred reactor. Thus, these expressions assume perfect mixing. In a gas-turbine combustor, however, regions of unmixed species will exist, and turbulence will also influence the soot production rates. As such, modifications to these expressions are required before they can be used for a general 3-D turbulent flow.

3.5.3 Influence of Turbulence on Soot Formation and Oxidation

Magnussen, et al., 45,46 have proposed a model that accounts for the influence of turbulent fluctuations on soot production rates. In turbulent flows, chemical reaction occurs when reactants at a sufficiently high temperature are mixed at the molecular level. The molecular mixing process is analogous to the dissipation (ϵ) of turbulent kinetic energy k and is associated with the smallest scales of turbulence. Dissipation is concentrated in highly strained regions of the fluid occupied by fine structures with characteristic dimensions of the same magnitude as the Kolmogorov microscale. The reactants are molecularly mixed in these fine structures, where reaction occurs. Magnussen, et al., proposed the following expressions for the mass fraction contained in the fine structures:

$$\gamma^* = 9.7 \cdot (R_1) \tag{119}$$

where \mathbf{R}_{t} is the turbulence Reynolds number, and the rate of transfer of mass per unit mass between the fine structures and the surrounding fluid is

$$\dot{m} = 23.6 \cdot (R_{\dagger})^{-1/4} \frac{\epsilon}{k} \tag{120}$$

The rate of reaction is proportional to $\dot{m} \chi$ where χ is the fraction of small-structure eddies that are sufficiently heated to react. It is assumed that χ is proportional to the ratio of local reacted fuel concentration and total fuel concentration. Thus, the rate of reaction is

$$R_{fu} = 23.6 (R_f)^{-1/4} \frac{\epsilon}{k} \chi C_{min} (kg/m^3.s)$$
 (121)

where

$$X = \frac{C_{pr}/(1+i)}{C_{pr}/(1+i) + C_{fu}}$$

$$C_{pr} = \text{Product concentration}$$

$$C_{fu} = \text{Fuel concentration}$$
(122)

 C_{\min} is the smaller of C_{fu} and $(C_{\mathrm{O2}}/\mathrm{i})$ and i is the stoichiometric oxygen requirement. The temperature T* of the reacting fine structures is T above the local time-mean temperature T:

$$T* = T + \Delta T = T + \frac{\Delta H_R C_{min}}{\rho C_{p}}$$
 (123)

where:

$$H_R$$
 = the heat of reaction C_p = the specific heat.

and the surrounding temperature T° is

$$T^{O} = T - \Delta T \left(\frac{\gamma * \chi}{1 - \gamma * \chi} \right). \tag{124}$$

Using Equations (107) and (109), the mean rates of nuclei and soot formation are then expressed as

$$R_{n,f} = n_{o,T*} \cdot \gamma^* \cdot \chi \cdot \rho/\rho^* + n_{o,T^o} (1 - \gamma^* \cdot \chi) \cdot \rho/\rho^o + (f - g) n$$

$$-g_o n^* N^* \gamma^* \chi \rho/\rho^* - g_o n^o N^o (1 - \gamma^* \chi) \rho/\rho^o$$
(125)

and

$$R_{s,f} = m_{p} (a - b N^{*}) n^{*} \gamma^{*} \chi \rho / \rho^{*}$$

$$+ m_{p} \cdot (a - b \cdot N^{0}) \cdot n^{0} (l^{`} - \gamma^{*} \chi) \cdot \rho / \rho^{0}$$
(126)

Finally, the mean rates of nuclei and soot oxidation are expressed as:

$$R_{n,c} = R_{fu} n/C_{fu} (part/m^3 s)$$
 (127)

$$R_{s,c} = R_{fu} C_s/C_{fu} (kg/m^3 s)$$
 (128)

Magnussen, et al., used this model to compute the soot concentrations in a turbulent C_2H_2 diffusion flame. By adjusting the particle diameter [entered as m_p , the particle mass in Equation (109)], and the constant a_0 in Equation (107), good agreement with experimental measurements was obtained.

3.5.4 The Garrett Soot-Emission Model

The model adopted by Garrett for computing soot emissions under NASA Contract NAS3-22542 is described in the following paragraphs.

The computation of soot emissions involves the solution of two additional transport equations for the concentrations of nuclei and soot. To complete the equation specifications, the source terms and the Schmidt numbers for these two variables are as follows:

The source term for nuclei concentration is expressed as

where $R_{n,f}$ is given by the smaller of the two values from Equations (108) and (125), $R_{n,c}$ is given by Equation (127). Thus, these expressions amount to the use of the turbulent reaction rates, subject to the limitation that they cannot be greater than the rates under well-stirred reactor conditions.

The source term in the soot concentration Equation (111) is similarly expressed as:

where $R_{s,f}$ is given by the smaller of the two values from Equations (112) and (126); $R_{s,c}$ is given by the smaller of the two values from Equations (113) and (128).

The turbulent Schmidt numbers $\sigma_{\rm S}$ and $\sigma_{\rm n}$ for soot and nuclei concentrations are assumed the same as for gaseous fuel (i.e., 0.9).

This model has been incorporated into the Garrett 3-D combustor performance program. Preliminary computations indicate its ability to make qualitative predictions.

3.6 Radiation Modeling

An adequate treatment of radiative heat transfer from combustion products is essential for the prediction of gas-turbine liner temperatures and heat-transfer rates. For this purpose, Garrett is at present using the six-flux radiation model based on the Schuster-Hamaker approximation. The influence of soot, $\rm CO_2$, and $\rm H_2O$ on the radiation properties (absorptivities and emissivities) is included in these equations.

3.6.1 The Flux Methods

In the flux methods, the angular distribution of radiation intensities is replaced by a number of discrete intensity vectors in different directions, thus reducing the complexity of the integro-differential equation of radiation heat transfer. The energy transfer in each direction is represented by a closed firstorder ordinary differential equation obtained by integrating the radiation transfer equation over a solid angle. This method was originated for the 1-D case as the two-flux method, wherein only two directions are considered. Considerable errors exist in the two-flux solution in the case of essentially 1-D heat transfer between parallel plates; a situation for which the method is supposedly best-suited. This suggests that the two-flux method is not sufficiently accurate to permit its application to the prediction of radiant transfer in practical systems.

Spalding 48 extended the 1-D fermulation to two and three dimensions by formulating the four- and six-flux models. Extensions of the two-flux model to multi-flux and nongrey emitting absorbing media are also discussed by Siddall. 49 The four-flux model applied to an axisymmetric combustor underestimated wall radiation fluxes, although temperature predictions were reasonable. 50

The reasons for the inaccuracies in these flux methods are (a) the radiant flux is divided into too few directions (2, 4, or 6 being small for many applications or (b) the fluxes in the different directions are unrealistically independent of each other. Another limitation of the flux models is that their extension to general curvilinear coordinates for handling complex geometries is rather cumbersome.

3.6.1.1 The Six-Flux Model Used at Garrett

A six-flux radiation model based on the Schuster-Hamaker approximation 47 is used currently at Garrett. It should be noted that, as pointed out by Siddall 49, other flux model approximations such as Milne-Eddington and Schuster-Schwarzschild can be represented by the same form of flux equations with constants being different.

The differential equations describing the variations of the fluxes along six directions can be reduced to the following three second-order ordinary differential equations:

$$\frac{d}{dx}\left(\frac{1}{a+s} - \frac{dR^{X}}{dx}\right) = a\left(R^{X}-E\right) + \frac{s}{3}\left(2R^{X} - R^{T} - R^{Z}\right)$$
 (129a)

$$\frac{1}{r}\frac{d}{dr}\left(\frac{r}{a+s+\frac{1}{r}}\frac{dR^{r}}{dr}\right) = a\left(R^{r}-E\right) + \frac{s}{3}\left(2R^{r}-R^{x}-R^{z}\right)$$
(129b)

$$\frac{1}{r}\frac{d}{d\theta}\left(\frac{1}{a+s}\frac{dR^{Z}}{rd\theta}\right) = a\left(R^{Z}-E\right) + \frac{s}{3}\left(2R^{Z}-R^{X}-R^{r}\right) \qquad (129c)$$

Where the composite-fluxes R^{X} , R^{r} and R^{Z} are defined as

$$R^{x} = \frac{1}{2} (I_{x+} + I_{x-})$$

$$R^r = \frac{1}{2} (l_{r+} + l_{r-})$$

$$R^{Z} = \frac{1}{2} \left(I_{\theta+} + I_{\theta-} \right)$$

where I_{x+} , I_{r+} and $I_{\theta+}$ are the fluxes along the positive directions of axial, radial, and circumferential directions, respectively; I_{x-} , I_{r-} , and $I_{\theta-}$ are the corresponding fluxes along the negative directions.

- a = absorption coefficient, defined as radiation absorbed
 per unit length
- s = scattering coefficient, defined as radiation scattered
 per unit length
- $E = black body emissive power = \sigma T^4$
- σ = the Stefan-Boltzman constant.

3.6.2 Discrete Transfer Method

Lockwood and Shah⁵¹ have presented a method called the discrete transfer method. This method is based on the solution of representatively directed beams of radiation within the combustor, as in the Monte Carlo method. However, in this method the directions of the rays are specified in advance and they are solved for only between two boundary walls contrary to the Monte Carlo method where the ray directions are specified at random and the rays are tracked to extinction. Lockwood and Shah have shown that this

method closely reproduces the analytical solution for radiation between parallel plates (1-D case), radiation in a square enclosure (2-D), and in a cubic enclosure (3-D). The conventional two-, four-, and six-flux models for these cases show larger errors. This new method is economical, geometrically adaptable, provides ease of application, and has the possibility of obtaining any degree of precision (through the specification of number of rays). The method is designed to be coupled to fluid flow solutions. GTEC has used this method in its 2-D combustor program.

3.6.3 Radiation Properties

The contributors to radiation fluxes in gas turbine combustors are: soot, ${\rm CO_2}$, ${\rm H_2O}$ (vapor), inorganic particles, etc. Only the influence of soot, ${\rm CO_2}$, and ${\rm H_2O}$ (vapor) is discussed here. Although CO and unburned ${\rm C_xH_y}$ contribute to emission and attenuation of radiation within flames, these contributions are localized and of secondary importance for computing radiative fluxes. The contributions of ${\rm NO_x}$ and ${\rm SO_2}$ can be neglected because of their low concentrations.

The radiation properties of the principal radiating species including soot, CO₂, and H₂O are significantly nongrey. Consequently, the calculation of the radiation properties is a time-consuming task. However, detailed spectral calculations are unnecessary since approximate calculations (by means of curve fits) are more convenient and provide good accuracy. Garrett has employed the approximate curve-fit procedure for the calculation of radiation properties under NASA Contract NAS3-22542.

The absorptivity (α) of the gas-soot mixture includes the soot absorptivity, the absorptivity due to the absorption bands of CO₂, and H₂O and corrections for the overlapping of bands.

Using the spectral data, 53 the gas absorptivity is calculated by taking a summation over the absorption bands of CO $_2$ and H $_2$ O. In the approximate calculation method adopted by Garrett, a simpler approach is used. The gas absorptivity, $\alpha_{\rm q}$ is written as 54

$$\alpha_g \epsilon_g (T/T_s)^{(0.6-0.2\zeta)}$$

where
$$\zeta = P_W/(P_W + P_C)$$

 $\epsilon_{
m q}$ = gas emissivity at a temperature T and path length LT_s/T

 P_{C} , P_{W} = partial pressure of CO_{2} and $H_{2}O$

$$\epsilon_g = \epsilon_C + \epsilon_W - \Delta \epsilon_{CW}$$

where

 $\epsilon_{\rm C}$, $\epsilon_{\rm W}$ = emissivities of ${\rm CO_2}$ and ${\rm H_2O}$

 $\Delta \epsilon_{CW}$ = overlap correction factor.

 $\epsilon_{\rm g}$ can be computed using a temperature adjusted version of Leckner's approximate overlap correction $\Delta \epsilon_{\rm CW}$, and approximating $\epsilon_{\rm C}$ and $\epsilon_{\rm W}$ by curve fits of P_C, P_W, T and path length to spectral calculations. In the range of interest in gas-turbine combustors, such calculations agree to within 5 percent of the spectral calculations and the experimental results. The absorptivity (α) of the gas-soot mixture is given by

$$\alpha = \alpha_s + \alpha_g - \alpha_s \alpha_g$$

With $\alpha_{\rm g}$ obtained above, it remains to determine $\alpha_{\rm s}$, the soot absorptivity. This is obtained by the method of Felske and Tien. ⁵⁶ This method assumes that the complex refractive index of soot is independent of wavelength and that the soot particle diameter is small compared to the wavelength of radiation, so that scattering is negligible. The spectrally integrated absorptivity can then be written in a closed-form expression to determine $\alpha_{\rm s}$.

By using the radiative property calculations of the type described above, Sarofim⁵⁷ indicated that radiation calculations can be made with fair confidence, and that the major source of uncertainty in such calculations is soot concentration, rather than gas-radiaton properties.

SECTION IV

4.0 DESCRIPTION OF THE COMPUTATIONAL SCHEME

The governing differential equations described in Section 3.0 are nonlinear and coupled partial differential equations. In most practical situations, it is not possible to obtain analytical solutions to these equations and numerical methods have to be used. A description of the numerical scheme used in the CPM is provided in Paragraph 4.1. The treatment of the boundary conditions is given in Paragraph 4.2, and the criteria for convergence and the method for assessing grid independence are outlined in Paragraph 4.2.

4.1 Description of the Numerical Method

The numerical method used in the CPM's are based upon the finite difference technique of Patankar, ⁵⁸ which used the Semi-Implicit Method for Pressure Linked Equation (SIMPLE) algorithm. The features of this computational procedure include the following:

- Solution of a sufficiently general single form of differential equations
- o Provision for use with different physical models
- o Use of pressure and velocities as the main hydrodynamic variables
- o Use of the pressure-correction technique
- O Use of nonuniformly spaced grids
- o Use of staggered storage locations

- o Derivation of finite-difference equations by integrating the differential equations over finite control volumes
- o Line-by-line solution of the difference equations

The finite-difference equations are derived for a box-shaped flow domain. Over the region of interest, a number of grid planes parallel to the two coordinates are placed. For each grid node, the finite-difference equations are set up for each of the flow variables to be solved. Since the governing equations for axial-and radial-velocities (Equation 1) contain pressure gradient terms, these two variables are solved along planes staggered with respect to the main grid planes described above.

A typical grid node spacing for a general flow problem is shown in Figure 4.1-1. Finite-difference equations for a node are obtained by integrating the differential equations over a control volume enclosing a grid node. For evaluating the convection and diffusion fluxes through a control volume face, a linear variation (in the direction normal to the face) of the flow properties is assumed. For other purposes, a stepwise variation with discontinuities at control-volume boundaries is assumed. Net rate of flow of ϕ into the control volume around a node P (Figure 4.1-1) by convection and diffusion in the x-direction is

$$[T_{X-} + (1 - f_{X-}) L_{X-}] \phi_{X-} + [T_{X+} - f_{X+} L_{X+}] \phi_{X+}$$

$$-[T_{X-} - f_{X-} L_{X-} + T_{X+} + (1 - f_{X+}) L_{X+}] \phi_{P}$$
(130)

where

$$T_X = \Gamma_{eff,\phi} A_X / \delta X$$

$$L_{X} = m_{X}^{"}/\delta X$$

$$A_{X} = 0.5 (r_{+} + r_{-}) \Delta Y$$

. Defining $\int \int \int S_\phi dV = S_u + S_p \phi_p$, the one-dimensional transport equation for the variable becomes

$$[T_{X-} + (1 - f_{X-}) L_{X-} + T_{X+} - f_{X+} L_{X+} - S_p] \phi_p$$

$$= [T_{X-} + (1 - f_{X-}) L_{X-}] \phi_{X-} + [T_{X+} - f_{X+} L_{X+}] \phi_{X+} + S_u$$

(131)

The linear-profile assumption becomes unacceptable when f_{X+} L_{X+} is large compared with T_{X+} because with weighting factor $(T_{X+} - f_{X+} L_{X+})$ then becomes negative, implying an unrealistic physical process through which raising the value of ϕ_{X+} could lower the value of ϕ_{p} . Therefore, it is assumed that if the convective flow rates (L) are large compared to the diffusion coefficients (T), the diffusion across the control-volume face is zero and the value of convected is equal to the value at the node on the upwind side of the face. With this assumption, the coefficient $T_{X+} - f_{X+} L_{X+}$ is replaced by $T_{X+}^* - F_{X+} L_{X+}$ where

$$T_{X+}^* = [T_{X+}, -(1 - f_{X+}) L_{X+}, f_{X+} L_{X+}]$$

Here $[a_1, a_2, a_3]$ stands for the largest of the three quantities a_1, a_2 , and a_3 .

Using a similar procedure for the fluxes in the radial direction, the final finite-difference equation is reduced to

$$A_{p}^{\phi}_{p} = A_{X_{+}^{\phi}X_{+}} + A_{X_{-}X_{-}} + A_{Y_{+}^{\phi}Y_{+}} + A_{Y_{-}^{\phi}Y_{-}} + S_{u}$$
(132)

The solution of the above equation is obtained by line-by-line relaxation using an efficient tri-diagonal matrix algorithm. By this method, a traverse along one direction, for example, the X-direction, is made with old values for the y-direction nodes. Using this solution as the best estimate, the y-direction is then traversed. The solution method adopted is based on the SIMPLE algorithm of Patankar and Spalding as described in Reference 15.

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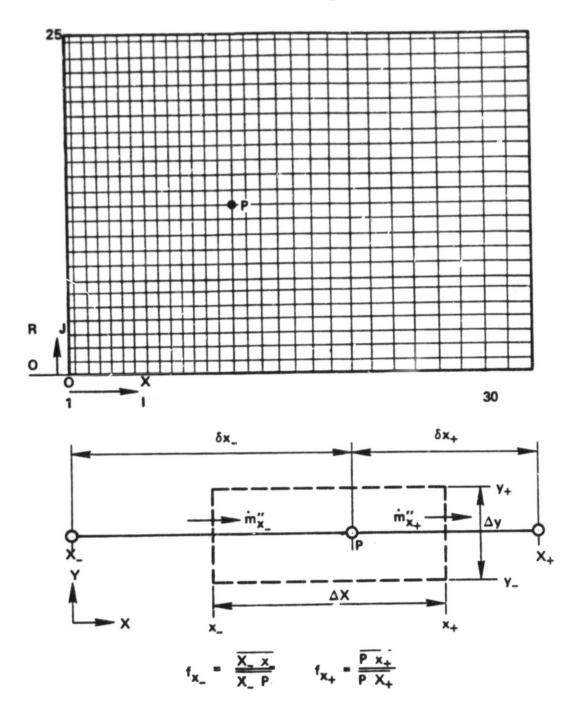


Figure 4.1-1. Typical Grid Spacing of the Swirling Flow Problem and Control Value around a Point P.

4.2 Boundary Conditions

The boundary conditions are enforced by appropriately modifying the finite-difference coefficients at the first interior point adjacent to the boundary. For the inlet boundaries, the velocity components, density, and turbulence profiles are either experimentally known or estimated. At the inlet boundary, if pressure is specified, the pressure correction is set to zero. When the normal velocities at the boundary point are specified, the coefficients in the pressure correction are modified in such a way that the mass fluxes through the control volume satisfy the overall continuity equation.

For boundaries of the second kind, where gradients and not the values of the variables are specified, the program uses one of the following two approaches. In the first approach, the boundary value is guessed and continually updated to satisfy the given gradient condition. The second approach breaks the link through the boundary to all adjoining external control volumes by first arranging for the finite-difference coefficient connecting the boundary node to an internal node to be zero, and then inserting the correct flux at the boundary as a source of diffusion and/or convection for that internal node.

At the symmetry plane, the convection and diffusion fluxes in the radial direction are zero. Therefore, the finite-difference coefficients containing these fluxes are set to zero at the axis of symmetry. For the exit plane, information about some of the variables is not available. However, since it is the process occurring in the calculation domain that decides values of the variables that the outgoing fluid will carry, there is no need for information at such boundaries. These boundaries are simply treated by neglecting the diffusion at the exit boundary.

Boundary conditions at the near-wall nodes are treated in the manner outlined in Section 3.0 (Equations 7 through 9).

The input parameters depend upon the nature of flow problem computed. In many of the test cases, initial profiles of turbulence kinetic energy (k) and length scales (L) are not available. For these cases, uniform profiles of k and L are prescribed at the inlet and the default values used are

$$k = 0.003 u_{av}^2$$

$$L = 0.02 R_{max}$$

where, $U_{\rm av}$ is the average inlet velocity, and $R_{\rm max}$ is the maximum cross-stream dimension of the flow geometry. If information about turbulence intensity levels is available at the inlet, appropriate uniform k values are used at the inlet.

4.3 Convergence Criteria

The solution is accepted as the converged solution when the total mass source error is less than about 0.1 percent of the total mass flow rate. For all the test cases, the computations were carried out further to ensure that the profiles of the dependent variables did not appreciably change. For all the test cases considered in this program, when the solution converged to the acceptable limit of 0.001 on the total mass source error, the maximum mass source error in the computational domain was less than 0.0002. The number of iterations required to reach the acceptable convergence level varied from problem to problem. In most of the recirculating flows, a minimum of 350 iterations were needed to reach the convergence criterion.

During the computations, the values of each dependent variable are monitored to ensure that the maximum change in the value of each dependent variable is a small fraction of the reference value. When this condition is satisfied, and if the total mass source error is less than 0.1 percent, plots of all the variables of interest are obtained. Computations are then continued for another 50 iterations and plots are obtained again. If these plots are identical to within graphical accuracy, the solutions are accepted as converged solutions.

The numerical solution obtained for any given flow problem depends upon the grid density and grid distributions. The solutions are accepted as grid independent if the predicted results are essentially invariant when the grid density or the grid distributions are changed. This type of test was performed for many of the test cases, but these test results will be presented only for a few of them. For the other cases, the predictions presented in this report are essentially grid independent. The details about the grid distributions for each test case will be provided along with the discussion of the results.

SECTION V

5.0 DATA BASE FOR BENCHMARK QUALITY TEST CASES

To assess and critique the current models and generate a program plan to improve their accuracy and usefulness as a combustor design tool, the assessment of the models was conducted in the following two interrelated steps:

- Assess and critique the physical submodels involving the fundamental processes of combustion, individually, with data from ideal element tests under well-defined conditions. The physical submodels considered here are turbulence modeling, gaseous fuel combustion, spray evaporation and combustion, soot formation and oxidation, and radiation modeling.
- o Assess and critique the model predictions against the data from advanced gas turbine combustors.

Accordingly, the data base is arranged in two sections: Paragraph 5.1 includes a description of the data base from ideal element tests and Paragraph 5.2 contains a description of the data from a number of gas turbine combustors.

5.1 Data Base from Ideal Element Tests

A literature survey of recently published work (generally 1970 or later) was conducted to compile a data base necessary for a benchmark quality test case. Published literature related to the following submodels was reviewed:

- o Turbulence Modeling
- o Gaseous Fuel Combustion
- o Spray Evaporation and Combustion
- o Soot Formation and Oxidation

In the following paragraphs, a data base from ideal element tests is provided. The ideal tests range from simple entrance flows in pipes and 2-D channels to more complex flows like the flow fields behind steps, blockages, and swirling recirculating flows. These tests are intended to encompass the range of complexities involved in combustor internal flows. Simple entrance flows are included in the validation efforts to ensure that the analytical models can be used to predict simple flows without any modification to the model. The data base selected has fairly detailed measurements, including turbulence parameter measurements, with estimations on errors.

5.1.1 <u>Turbulence Modeling</u>

In this paragraph, a data base for assessing turbulence models is provided. The assessment procedure for the k-f turbulence models will consist of comparing the predicted time-mean velocity components with the corresponding measurements. For the algebraic and full Reynolds stress models, the predictions of the turbulence intensities and cross correlations will also be compared with the measurements. Some cases involving scalar transport are also considered, and these involve predictions of the concentration of a trace gas (inert) or temperature under heated but inert conditions.

The references reported in the following tables provide information about the available measurements reported in the literature.

These references were selected based upon the extent and accuracy of the data and the nature of the geometry of test conditions. The references selected are presented in the form of increasing order of complexity of the flow field in the form:

- o Simple Flows (Boundary Layers, Jets, Mixing Layers, etc.)
 (2-D Parabolic) Table 3
- o Streamline Curvature Effects (Curved Ducts, Curved Boundary Layers, etc.) (2-D Parabolic) Table 4
- o Recirculating Flows (Nonswirling) (Both Unconfined and Confined) (2-D Elliptic) Table 5
- o Swirling Flows (With and Without Recirculation) (2-D Elliptic/2-D Parabolic) Table 6
- o Scalar Transport Table 7.

From the references provided in these tables, benchmark test cases were selected, as described in Sections 6.0, 7.0 and 8.0. These cases were used to evaluate the turbulence and kinetic model predictions.

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FLOW FIELD HAS PECIRCULATION REGIONS REMARKS FLOW IS UNCONFINED ORIGINAL PAGE IS OF POOR QUALITY INITIAL CONDI-TIONS WELL OTHERS 3 NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES <u>*</u> 4 S SIMPLE FLOWS (CONTD). **1** ₹ 2 2 S **~** 12 S ထ WELOCITY S œ NUMBER OF TEST CASES ئ TABLE JET INTO COFLOWING FREE STREAM GEOMETRY AND MEASUREMENT TECHNIQUES DISA SINGLE HOT WIRE PROBES (2-D ELLIPTIC) CONFINED COAXIAL JET (2-D PARABOLIC) HOT WIRE (2-D PARABOLIC) HOT WIRE 1 1 1 HABIB, M.A. AND WHITELAW, J.H. (1979) REF. 62 SMITH, D.J. AND HUGHES (1977) REF. 63 CHAMPAGNE E.H. & & WYGNANSKI 1.J. (1970) REF. 64 AUTHOR (YEAR) CASE SECTION 6.7

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DATA INCLUDE COMPUTED VALUES OF BOUNDARY LAYER INTEGRAL PARAMETERS DATA INCLUDES 1 CASE WITH NO SUCTION, ALL OTHER CASES HAVE SUCTION CASE H612 OF STANFORD CONFERENCE REMARKS TURBU-LENCE INTEN-SITY SITY INITIAL CONDI-TIONS OTHERS LENGTH CLAU-SER PLOTS ∞<u>8</u>₩ NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES > ဆ 7.M |~ |-> -œ **⊳** 88 WEAN ន ~ œ NUMBER OF TEST CASES ജ 2 *€munumhhmmm* × MEASUREMENTS USING A RAKE OF PRESSURE PROBES. GEOMETRY AND MEASUREMENT TECHNIQUES HOT WIRE (2-D PARABOLIC) DEVELOPING DUCT FLOW (2-D PARABOLIC) (2-D PARK新宝器) WATTS, K.C. AND BRUNDPETT, E. (1979) EMERY, A.F. AND GESSNER, F.B. (1976) SECTION 6.3 WIEGHARDT, K. AND TILLMANN, W. (1944) REF. 66 SECTION 6.1 AUTHOR (YEAR) REF. 67 REF. AS CASE

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TABLE 3.

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TURBULENCE IS ANISOTROPIC.
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PROFILES ARE GIVEN AT REMARKS X 0 =-.05 INITIAL CONDI-TIONS A A B E E E YES OTHERS **NUMBER OF MEASUREMENT LOCATIONS** LC) TURBULENCE PROFILES -9 A.S 9 9 , A RECIRCULATING FLOWS. 9 9 16 15 25 120 € 9 = 8 € MEAN 9 9 13 28 CASES WITH Red_n= 3500 – 28,300 NUMBER CASES TEST 뇸 ĺζ, minimal minima PULSED WIRE ANEMOMETER MEASUREMENTS (2-D ELLIPTIC) TABLE GEOMETRY AND MEASUREMENT TECHNIQUES BACKWARD FACING STEP LDV MEASUREMENTS L.DA MEASUREMENTS (2-D ELLIPTIC) FRUNT FACING STEP **AXI-SYMMETRIC** (2-D ELLIPTIC) 2 D FENCE 1111111 5 D.F.G DURAD AND J.H WHITELAW" (1978) REF. 78 W.D. MOSS AND S. BAKER: (1980) R. SMYTH (1979) REF. 77 REF. 79 AUTHOR (YEAR) CASE

UNCENTAINTY ABOUT FLOW STEADINESS AND THREE GAMENSONALIY. THE AMOUNT OF DATA IS LIMITED COMPARED TO STANFORD WORK, SIMILARITY PROFILES FOR Ü
AND TRACER GAS CONCENTRATIONS DOCUMENTATION IN REATTACHED LAYER IS GOOD PRESSURE DISTRIBUTION ON UPL'ER AND LOWER WALLS AVAILABLE. REMARKS INITIAL CONDI-TIONS OTHERS ن NUMBER OF MEASUREMENT LOCATIONS 9 .<u>~</u> TURBULENCE PROFILES 'n RECIRCULATING FLOWS (CONTD). 1° H s ഗ 12 9 S 120 ~ 5B က MEAN VELOCITY 2 6 S CASES TEST 片 folet settling screen MEAN VELOCITIES USING PITOT PROBE AND FLOW ANGLES WITH RICARDO PROBE. ALSO TRACER GAS SAMPLING STUDY. IJ, 9 LDV MEASUREMENTS FOR h = 101.6 MM, $R_{\text{eh}} = 168,000$. TABLE GEOMETRY AND MEASUREMENT TECHNIQUES 5 (2-D ELLIPTIC) (2-DELLIPTIC) (2-DELLIPTIC) HOT WIRE VELOCITY MEASUREMENTS Reh. = 45,000 $R_{e_0} = 50,000$ R. BREMMER, H.D. THOMPSON AND WH. STEVENSON-(1980) W.H. SCHOFIELD AND T.S. KEEBLE (1974) J. KIM. S.J. KLINE AND J.P. JOHNSTON-(1978) SECTION 7.2 REF. 80 REF. 82 AUTHOR (YEAR) CASE

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STREAMLINE AND ISOBAR CONTOURS ARE AVAILABLE. FLOW IS UNCONFINED. \$\psi\$ THE STREAM FUNCTION. CONTINUATION OF EFFORT BY KIM, ET. AL. REMARKS DATA IS VERY LIMITED. WELL INITIAL CONDI-TIONS Ü Aĭ X = 0 OTHERS ج ہ NUMBER OF MEASUREMENT LOCATIONS RECIRCULATING FLOWS (CONTD). TURBULENCE PROFILES) |-6 ¥.5 5 ŝ 2 2 3 **~ 5 注** MEAN VELUCITY ß 5 5 6 b NUMBER CASES OF TEST $Re \theta = 240$ 510 8505 TABLE GEOMETRY AND MEASUREMENT TECHNIGUES VELOGITY MEASUREMENTS USING PITOT TUBES. (2-D ELLIPTIC) (2-D ELLIPTIC) 12-D ELLIPTIC) PLANE FLOW LOV MEASUREMENTS, COAXIAL JETS. (O IS THE MOMENTUM THICKNESS) (December of the last of the l PULSED WIRE ANEMOMETER † Red = 150,000J.K. EATON AND J.P. JOHNSTON (1980) SECTION 7.2 N.A CHIGIER AND J.M. BEER (1964) REF. 85 AUTHOR (YEAR) REF. 83 F.K. OWEN (1976) REF. 84 CASE

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SIZE AND MASS OF RECIRCULATION Zone. Good estimates of Biasing Enrors. S" = DISPLACEMENT THICKNESS MEASURED PROFILES SHOW NO RECIRCULATION. DATA MAY BE QUESTIONABLE. WORKING FLUID IS WATER. P.D.F. SKEWNESS & FLATNESS ARE AVAILABLE. REMARKS 2 5 A INITIAL CONDI-Tions OTHERS SKEW-NESS AND FLAT-NESS NUMBER OF MEASUREMENT LOCATIONS RECIRCULATING FLOWS (CONTD). TURBULENCE PROFILES <u>}</u> 9 ¥. ~ - A 4 ເລ **~~~** 12 c ~ > 5 ≥ MEAN VELOCITY **~~~** _ 2 CASES WITH Re = 15,900 AND 47,500 R_{eH}= 1.5x10° 2.2x10°= 3.7x10°= NUMBER CASES OF TEST 0.06 0.08 0.23 LBV MEASUREMENTS WITH AND WITHOUT CHEMICAL REACTION 5. HOT WIRE MEASUREMENTS. ($C_{td}\!=\!c_{RAYA}$ -Curtet number) ++++ 1111 GEOMETRY AND MEASUREMENT TECHNIQUES LDV/LIF MEASUREMENTS. (2-D ELLIPTIC) (2-DELLIPTIC) (2-D ELLIPTIC) H = 51mm **†|†**|†|†| B.V. JOHNSON AND J.C. BENNETT SECTION 7.8 K. GÜRÜZ AND C. ILICALI? (1961) SECTION 7.7 R.W. PITZ-(1981) REF. 86 AUTHOR (YEAR) CASE REF. 88

TABLE

U. u'v', k, € & µt with blowing at 4 axial, planes. Similarity profiles for Mean velocity field ONLY MEAN VELOCITY PROFILES ARE REPORTED. REMARKS INITIAL PROFILE WITHOUT THE RINS INITIAL CONDI-TIONS | e | e EXEW-XESS NESS NESS OF PROBABI-LITY FUNC OTHERS (CONTD). NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES <u>-</u> -RECIRCULATING FLOWS 1 * 4 **!**-**⊳** ≥ 8 MEAN VELOCITY က 9 G RING CONFIGS. 9 NUMBER OF Test Cases S. LDV MEASUREMENTS AND TRACER GAS CONCENTRATION SAMPLING. TABLE Re = 280,000 LOV MEASUREMENTS. GEOMETRY AND MEASUREMENT TECHNIQUES (2-DELLIPTIC) (2-D ELLIPTIC) HOT WIRE MEASUREMENTS Re = 50,000 P. PHATARAPHRUK AND E. LOGAN: (1979) REF. 91 SECTION 7.4 I. F. MOON AND G. RUDINGER SECTION 7.3 SECTION 7.5 S. FUJII. M. GOMI AND K. EGUCHI' (1978) REF. 89 REF. 98 AUTHOR (YEAR) CASE

TABLE 5. RECIRCULATING FLOWS (CONTD).

			REMARKS	IMTIAL PROFILES ARE WELL Defined,	To The State of State			ORIGINAL PAGE IS OF POOR QUALITY
	\int	INITIAL	CONDI-	A! X=-1mm	•	*		
			OTHERS					
	DCATIONS	OFILES	. A.					
· (GIVE)	NUMBER OF MEASUREMENT LOCATIONS	TURBULENCE PROFILES	; _k		····	·		
	JF MEASUR	TURBUT	12.					
	NUMBERO		15	2				
		VELOCITY	5B				-	
		NEG E	139	9				
	NUMBER	OF TEST	CASES	4 MASS FLOW RATES.		<u> </u>	-	
	GEOMETRY AND			Screen Honeycomb	Centerbody Fuel Line Duct	LOV MEASUREMENTS BEHIND AN AXI SYMMETRIC BODY WITH AND WITHOUT INJECTION OF INERT GAS.	(2-0 ELLIPTIG)	
CASE	AUTHOR	(YEAR)	M. ROQUEMORE et.al. (1981)	REF. 92 SECTION 7.6		N.		
20								

UN CONFINED P. 574 DAIA FOR U AT X/D - 1, G, 17, 20, 20, 30, 8, 44 W PROIT (S. A. W) PROIT (S. A. Z) U - 6, 12, 8, 20 U - 7, A X/D - 6, 12, 8, 20 NO RECIRCULATION DATA PRESENTED IN ISOPLETH CONTOUR PLOTS FLOW FRED IS UN-CONFINED, WITH RECIRCULATE Y SWIRL NUMBER IS VERY HIGH. REMARKS UN-CONFINED FLOW. ALL PRO-FILES AT X=0 CONDI-TIONS OTHERS 图~ NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES 1 4 3 SWIRLING FLOWS. -4 3 1 4 |>|<u>€</u>|c >> ≥ B MEAN ~ 9 NUMBER CASES OF TEST 9 TABLE Arrangment of coaxial jet, Vertical lines represent measurement stations. GEOMETRY AND MEASUREMENT TECHNIQUES MEASUREMENTS WITH HOT WIRE ANEMOMETER (2-D PARABOLIC) (2-D PARABOLIC) (2.0 ELLIPTIC) SWIRL NO. 0.26 SWIRL INDUCED BY ROTATING PIPES HOT WIRE MEASUREMENTS HOT WIRE MEASUREMENTS TANGENTIAL PORTS B.D. PRATTE AND J.F. KEFFER: (1972) Réf., 93 M. M. RIBIERO AND J. W. WHITELAW: (1980) REF. 94 N. SYRED, J.M. BEER AND N.A. CHIGIER: (1971) REF. 95 AUTHOR (YEAR) CASE

ANOTHER TEST CASE WITH BAFFLE AT THE EXIT OF THE TEST SECTION, INLET VELOCITIES ARE SMALL IN MAGNITUDE REMARKS INITIAL Condi-Tions OTHERS NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES 1 |~ ¥ 10 SWIRLING FLOWS (CONTD). ~ 9 12 6 > 5 B 요유 MEAN VELOCITY တ NUMBER OF TEST CASES 7 9 Schematic diagram of the yorks jube (linear dimensions in mm). TABLE 33 M/S REF VEL GEOMETRY AND MEASUREMENT TECHNIQUES LDV MEASUREMENTS (2-D ELLIPTIC) LDV MEASUREMENTS AND FLOW VISUALIZATION (2-D PARABOLIC) CONFINED SWIRL-DRIVEN FLEW -t-208,5 Synth (12) M/5 | 110 M/5 | -45° SWIRLER M.P. ESCUDIER, J. BORNSTEIN AND N. ZEHNDER: (1980) ALTGELD, H, JONES, W.P., AND WILHELMI, J. (1983) SECTION 8.6 REF. 218 AUTHOR (YEAR) AEF. 96 CASE

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CONFINED FLOW NO RECIRCULATION U.W. AND PRESSURE DISTRIBUTIONS, ANNILUS FLORE MEAN VEL. PROFILES AVAILABLE AT X/R₁ = 0.1, 0.21, 1,05, 2.1, 3,15,4.2 AND 8,92. Red = 7.8x10*-1.05x10* Data aval able at x/0=0.5, 1, 1.5, 2, 8, 2.5 REMARKS Ū&₩ Aī X=0 F0R α=90° OVERALL A. Swific NO ENTIAL CONDI-TICNS OTHERS NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES 1 SWIRLING FLOWS (CONTD). 7. H 4 4 **-**17 ~ iSm 12~ MEAN ~ CASES WITH α = 45° AND α = 90° α = 0° 45° AND AND α = 0° 45° AND AND 70° 2 (CO-SWIRL COUNTER-SWIRL) VANE ANGLE OF 45° NUMBER CASES OF TEST MEAN VELOCITIES WITH DIRECTIONAL PITOT PROBE. TURBULENCE DATA WITH HOT-WIRE ANEMOMETERS. (2-D EI LIPTIC) 9 MEASUREMENTS USING 5 HOLE PRESSURE PROBE. ALSO FLOW VISUALIZATION WITH TUFTS AND SMOKE WIRE. TABLE VELOCITY MEASUREMENTS WITH PRESSURE PROBES AT $\chi=1.7,4.2,7.0,10.3,14.8,22.2.8,32.7$ GEOMETRY AND MEASUREMENT TECHNIQUES 7/0 (2-D PARABOLIC) (2-D ELLIPTIC) SWIRLER VANES Ş SWIRL VANE ANGLE WINLET TRE kin W-D.L. RHODE AND D.G. LILLEY AND D.K. MCLAUGHLIN (1982) B.T. VU AND F.C. GOUL DIN (1980) REF. 89 C.J. SCOTT AND D.R. RASK (1973) REF. 98 AUTHOR (YEAR) REF. 97 CASE

S=SWIR. NO. DATA AVALABLE
WITH AND WITHOUT COAXIAL OUTER
FLOW DATA ALSO ANALABLE
WITHOUT SWIRL. FLOW FIELD IS
UNCOMFINED. GEOMETRY SAME AS PHODE & LILLEY, TURBULENCE DATA GN SWRLING FLOW AVALABLE OMLY AI $\frac{X}{X}$ = 0.5, 1.0 8 1.5. COMPARISON OF DATA WITH PRIODE & LALEY'S DATA SHOW SOME DIFFERENCES IN W REMARKS ORIGINAL PAGE IS OF POOR QUALITY INITIAL CONDI-TIONS Aï X/0=0.5 OTHERS C'W' BEN4 NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES 34 တ က SWIRLING FLOWS (CONTD). * m |~ |-9 m 120 9 4 **⊳** 8 € **თ** ო WELDCITY SWIRL ANGLE 0° 38° NUMBER CASES OF TEST S=0.25 S=0.35 9 TABLE GEOMETRY AND MEASUREMENT TECHNIQUES MEASUREMENTS WITH HOT-WIRE ANEMOMETER. (2-D ELLIPTIC) MEASUREMENTS WITH HOT WIRE ANEMOMETER (2-D PARABOLIG) S.I.JANJUA DK.MCLAUGHLIN, T.W.JACKSON AND D.G.LILLEY (1982) RFF, 100 SECTION 8.5 AUTHOR (YEAR) CASE SECTION 8.1 A.P. MORSE (1980) REF. 101

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TABLE 6. SWIRLING FLOWS (CONTD).

		4000000	nemarka	ACCURACY OF DATA IS UNCERTAIN PROBE INTERFERINCE EFFEUS ARC UNKNOWN. SWBLER VANE ANGLES OF 15°, 30°, 45°, 60°, 70° AND 75°.	SOME UNICERTANTIES ABOUT STEADWESS, 3-DWENSIONALITY AND ACCURACY IN SOME REGIONS, SWIRLER VALVE AND ES OF 0°- 30°, 60° AND 60° WITH A RING.	MEASUREMENTS W.A CAN COMBUSTOR, NO TURBULENCE DATA.
		IKILIYE	TIONS	•	e €£	
ŀ			OTHERS	WALL STATIC PRESS.		
	OCATIENS	OFILES	<u> }</u>			
	JREMENT (WELOCITY TURBULENCE PROFILES	* <u>*</u>		us	
	NUMBER OF MEASUREMENT LOCATIONS		Z-A			
			12.	- production of the state of th	כנו	
			*8	2	, viii	G
-	l		1200	4	us	
	NUMBER	늉	test Cases	ي .	₹	-
		GEOMETRY AND MEASUREMENT TECHNIQUES		3-D PRESSURE PROBE SURVEY (2-D ELLIPTIC)	LOV MEASUREMENTS (2.0 ELLIPTIC)	3 HOLF PPR SSURE PRODE MEASUREMENTS.
	CASE	AUTHOR	(YEAR)	M.L. MATHUR AND N.R.L. MACCALLUM: (1967) RF, 102	GTEC (1981) RFF. 103 SECTION 8.3	GTEC (1901) Ref. 104 SECTION 8.2

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EXTENSIVE DATA_FLOW IS
RECHCULATING. C = AVG.
CONCENTRATION OF FLUORESCENT
DYS. FLUID MEDIUM — WATER DATA AVAILABLE IS VERY LIMITED. DATA IS VERY LIMITED. REMARKS INITIAL CONDI-TIONS U. V. AND AT X=0.25 OTHERS 54545-18° 1-4 E-NUMBER OF MEASUREMENT LOCATIONS -TURNULENCE PROFILES 7 _ SCALAR TRANSPORT. j~_ --WELOCITY 2 CASES WITH RB₆: 15,900 AND 47,500 OF TEST CASES 7. TABLE Re = 40,000 F?ye.wire measurements for fully developed Pipe Flon (2-d Parabolic) GEOMETRY AND MEASUREMENT TECHNIQUES (2-D PARABOLIC) LDV AND LIF MEASUREMENTS. (2-D EL LIPTIC) B.V. JOHNSON AND J.C. BENNETT (1981) REF. 88 J.F.KEFFER, G.J. OLSON AND J.G. KAWALL (1977) REF. 105 M. HISHIDA AND Y. NAGANA (1978) Ref. 106 AUTHOR (YEAR) CASE

TRIPLE CORRELATIONS SUCH AS $\overline{VU''}$, V'', VW'', V'', VW'', V'', VW'', DATA LIMITED TO FAR WAKE PAST RECIRCULATION ZONE DATA AVAILABLE ONLY IN THE SELF-SIMILAR REGION. REMARKS INITIAL CONDI-TIONS OTHERS SHE SHE SHE A.B. NUMBER OF MEASUREMENT LOCATIONS TURBULENCE PROFILES > SCALAR TRANSPORT (CONTD). .¥ ~ 2 চ ভ MEAN VELOCITY NUMBER CF TEST CASES HOT WIRE AND FINE-WIRE THERMOCOUPLE MEASUREMENTS. CONVENTIONAL AND CONDITIONAL SAMPLING DATA AT $\chi/D=15$. FAR WAKE OF A CYLINDER. FOUR WIRE PROBE MEASUREMENTS. AT X/D == 400 FULLY DEVELOPED TURBULENT BOUNDARY LAYER MAPPING WITH X WIRE ANEMOMETER AND FINE WIRE THERMOCOUPLE AT X = 47". 7. TABLE GEOMETRY AND MEASUREMENT TECHNIQUES (2-D PARABOLIC) (2-D PARABOLIC) FLOW D.S. JOHNSON (1959) Ref. 107 R. CHEVREY AND N.K. TUTU: (1977) REF. 108 AUTHOR (YEAR) G. FABRIS: (1977) CASE

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SCALAR TRANSPORT (CONTD). TABLE 7.

		REMARKS	INTERMITENCY OF TEMPERATURE FELD FOR INTERNAL AND EXTERNAL LAYERS ARE AVALLABLE.		ORIGINAL PAGE TO OF POOR QUALITY
		CONDI- TIONS			
		OTHERS			
RUZGER OF MEASUREMENT LOCATIONS	ROFILES	1	S		•
UREMENT	TURBULENCE PROFILES	F			
R OF MEAS	E	15	n		
SE SE	L	15	v		
	MEAN	- & B	ro.		
_	<u> </u>	-	up		
	NUMBER OF	TEST	-		
4	GEOMETRY AND	MEASUREMENT TECHNIQUES	minimum	3 HOT-WIRE ANEMOMETER MEASUREMENTS AT X = 70, 80, 90, 105 & 140 CM. (2-D PARABOLIC)	
CASE		AUTHOR (YEAR)	G. CHARIVAY, J.P. SCHON, E. ALCARAZ AND J. MATHEU (1977) REF. 110	Section 6.9	

5.1.2 Gaseous Fuel Combustion

In this paragraph, a data base for assessing gaseous fuel combustion models is provided. The assessment procedure consists of comparing the predictions of time-mean velocity components, temperature, concentrations of species (unburned fuel, CO, CO₂, H₂, H₂O, O₂, N₂) against the experimentally measured values of these quantities. These quantities were selected because they are of interest in gas turbine combustors. Reliable measurements of these quantities are available, and they are a good indication of the predictive capability of the gaseous combustion model consisting of the turbulence/chemistry interactions and the hydrocarbon reaction mechanisms. The assessment will be done for different flow types: turbulent/laminar, premixed/diffusion, one/two/three-dimensional flow, parabolic/elliptic, swirling/nonswirling.

In accordance with the assessment procedure, the data base is categorized into four sections:

- o Laminar Premixed Flames Table 8
- o Laminar Diffusion Flames Table 9
- o Turbulent Premixed Flames Table 10
- o Turbulent Diffusion Flames Table 11.

In each of these tables, the data is arranged in order of increasing complexity, starting from 1-D parabolic to 3-D swirling elliptic flows.

During the search for compiling the data base, several publications were encountered wherein the boundary conditions or other information required for modeling were not clearly or completely stated. Such cases (e.g., References 111-123) have not been included here. Measurements of quantities not related to the assessment procedure given above have also been excluded. The data base is concerned with the measurements of quantities listed above for steady gaseous hydrocarbon flames.

DATA USEFUL FOR VALIDATING 2 AND 4 STEP HYDROCAR-BON OXIDATION MECHINA-NISMS AND ESTABLISHING VALUES OF RATE CONSTANTS DATA USEFUL FOR VALIDATING 2 AND 4 STEP HYDROCARBON OXIDATION MECHANISMS AND ESTABLISHING VALUES OF RATE CONSTANTS. DATA USEFUL FOR VALOGING 2 AND 4 STEP HYDROCARBON OXDATION MECHANISMS AND ESTABLISHING VALUES OF RATE CONSTANTS THIS DATA WAS USED TO COMPARE 2 AND 4 STEP HY-DROCARBON OXIDATION MECHANISMS IN REF 153. REMARKS MEASUREMENT LOCATIONS ALONG FLAME AXIS ALONG FLAME AXIS ALONG FLAME AXIS ALONG FLAME AXIS COMPOSI-TYON ALONG FLAME AXIS ALONG FLAME AXIS ALONG FLAME AXIS TEMPERA-Ture OTHER QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE CO, CO₂, O₂, H₂O, C₄H_y OUARIZ MIC-ROPROBE AND MASS SPEC-TROMETER C3HB. CO. CO2. OUARTZ MICRO-PROBE AND MASS SPEC-TROMETER C₃H_B, CO, CO₂.
H₂, C₂H₄,
WAITER-COOLED
STANLESS
STEEL
SAMPLING
PROBE
AND GAS
CHROMATO
GRAPHY O2, CO, H2, CO2, H2O, OH, C₄Hy, LASER RAMAN SCATTERING COMPOSI-TION TEMPERA-Ture N₂ raman Spectrum THERMO-COUPLE THERMO. COUPLE TWO EQUIVA-LENCE RATIOS 3 EQUIVALENT RATKUS NUMBER OF CASES RICH, LEAN, STOICH, CH₄ AND STOICH, C₃H₈ RICH, LEAN And Stoich, C₃H₈-O₂ DILUTED WITH Ar. CH4-AIR AND CH4-02 CH4-AIR AND C3H8 - AIR C₃H_B - AIR FUEL 1-D PARABOLIC I D PARABOLIC I-D PARABOLIC 1-D PARABOLIC FLOW FLOW DESCRIPTION 1-D FLAT PREMIXED FLAME I-D FLAT PREMIXED FLAME PLUG FLOW REACTOR I-D PREMIXED FLAME SECTION 6.10 AUTHOR (YEAR) COOK AND SIMMONS (1982) HAUTMAN Et. al. REF. 125 CHANG AND TIERNAN: (1982) BECHTEL ET. AL. (1981) REF. 124 REF. 126 REF. 19

LAMINAR PREMIXED FLAMES

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TABLE

GARRETT HAS COMPUIED
THIS CASE WITH 2 STEP
HYDROCARBOW CARROW SOKEME AND ACREMENT
WITH DATA IS SHRY COCO
COMPUIATIONS WITH
4 STEP SCHEME REED TO
BE DONE RADIATION AND CONDUCTION CORRECTIONS TO TEMPERATURE MEASURE. INFLUENCE OF BUOY. ANCY IS IMPORTANT PEMARKS CONCENTRATION
MEASUREMENTS
ABSENT, DIRECT
ASSESSMENT OF
CHEMISTRY MODEL
NOT POSSIBLE. LIMITED AMOUNT OF DATA. RADIAL PROFILES OF AXIAL VELOCITY AT 3 AXIAL LOCATIONS CONTOUR PLOTS OF STREAM-LINES MEASUREMENT LOCATIONS COMPOSI-TION RADKAL PROFILES AY 3 AXIAL LOCATIONS ALONG FLAME AXIS TEMPERA-Ture RADIAL PROFILES AT 3 AXIAL LOCATIONS CONTOUR ALONG FLAME AXIS OTHER STREAM-LINES, VELOCITY, PARTICLE TRACKING AXIAL VELOCITY — LIJV QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE CO. CO2. O2. Fr. H20. UNCOOLED OUARTZ PROBE AND GAS CHROMATO-GRAPHY CH4, CO2, H20, O2, N2, CO - SAMP-LING PROBE AND FISHER-HAMILTON GAS PARTI-TIONERS. COMPOSI-TION TEMPERA-Ture THERMO-COUPLE THERMO-COUPLE THERMO-COUPLE 2 CASES FOR Different Air Velocities NUMBER OF CASES 뽕 뽏 뎚 MOIST CO - AIR CH4-AIR CH4-AIR 2-DELLIPTIC 2-DELLIPTIC 2-DELLIPTIC FLOW CONCENTRIC FUEL AND AIR JETS CONTAINED IN A VERTICAL CYLINDRICAL COMBUSTOR. OPPOSED JET DIFFUSION FLAME: FUEL O2 AND N2 Mixed and fed to the opposing burners Contained in a rectangular combuston Chamber. RECTANGULAR COMBUSTION CHAMBER WITH FUEL FED THRU A RECTANDULAR NOZZLE SUBROUNDED BY AIR. FLOW DESCRIPTION FUEL OXIDIZER N2 FUEL AIR -i SECTION 6.11 AUTHOR (YEAR) Kawamura Et, Al. (1980) Ref. 128 MITCHELL ET. AL. (1980) HAHN, WENDT AND TYSON (1981)

LAMINAR DIFFUSION FLAMES.

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TABLE

	REMAPKS		LIMITED ANOUNT OF DAILA AND THEREORE LIMITED UTRJIY	IM ET VELOCITY AND TURBULENCE RIVENSTY PROFILES MEASURED. PROVINES MEDIALE BOUNDARY CONDITION APUT	SAME SETUP AS PIZ AND DAUY, TOGETHERA DETAILED SET OF DATA IS AVALABLE
	TIONS	ОТИЕЯ	RADAL PROFIES OF VELOCITY AND TURBU- LEXES NITENSITY ANA ANAL LOCATIONS.	CROSS. SIPERM PROFILES OF AXIA. AXIAL LOCATIONS.	
	MEASUREMENT LOCATIONS	COMPOSI- TION			CROSS- STREAM PROFILES AT 4 AXIAL LOCATIONS
	MEAS	TEMPERA- Ture		,	CHOSS- STREAM PROFILES AT 4 AXIAL LOCATIONS
FLAMES.	ED AND Inique	ОТНЕВ	VELOCITY AND TURBU- TENCE INTENSITY - LDV.	VELOCITY COMPON- ENIS AND TURBU- LENCE INTENSITY - LDV.	
	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION			CO, CO;; SAMPLING PROBE, NON- DISPERSIVE INFRARED ANALYZEN. CHIP, FLAME DONISATION DETECTOR
PREMIXED	QUANJ	TEMPERA- Ture		·	COUPLE
TURBULENT	E	OF CASES	ONE	COLD AND HOT FLOW, WITH THREE REYNOLDS NUMBERS FOR EACH	HOT FLOWS
TURB	FUEL		CH4-AIR	C ₃ H ₀ - AIR	୍ଦେଖନ - ନାମ
E 17.	80 E	TYPE	2.0 ELLIPTIC	2.0 ELLPTIC	2.0 ELLIPTIC
TABLE	FLOW DESCRIPTION		2D COMBUSTION CHAMBER OF SOURE CROSS-SECTION PREMIXED FUEL + ARR HOT GASES FOR IGNITION	FLOW BEHIND A BACKWARD FACING STEP.	AS FOR PITZ AND DALLY
	AUTHOR	(YEAR)	MOREAU AND LABBE 11,2781 REF. 130	PITZ AND DOALY (1988) REF. 131	GANAI AND SANYER (1979) REF. 132 SECTION 7.8

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·	REMARKS	DISCUSSION ON ACCIRLLY OF MEASUREMENTS PROVIDED. VALIDATION FOR DIFFERENT FLOW CONDITIONS POSSIBLE	RADAL PROFILES OF AXAL VELOCITY AND TEMPERATURE MEASURED AT WALT - PROVINGS ACCURATE BOUNDARY CONOTION INPUT.	DATA PROVIDES FOR VALIDATION UNDER CONFINED PATABOLIC FLOW CONDITIONS.
TIONS	ОТНЕЯ		TOTAL PRESSURE -RADAL PROFILES AT 6 AXIAL LOCATIONS.	AXIAL VELOGIY -BADIAL PROFIES AYIAL LOCATIONS
MEASUREMENT LOCATIONS	COMPOSI- TION	AXIAL DISTRIBUTION ALONG CENTERLINE RADIAL DISTRIBUTION AT 4 AXIAL LOCATIONS		RADAL PROFIES A7.4 AXIAL LOCATORIS
MEAS	TEMPERA- Ture	AXIAL DISTRIBU- TIÓN ALONG CENTERLINE RJOAL DISTRIBU- TIÓN AT 4 AXIAL LUCATONS	RADAL FROFIES AT 8 AXIAL LOGATONS.	RADAL PROFILES AT 4 AXIAL LOCATIONS
ED AND INIQUE	ОТНЕВ		TOTAL PRESSURE. PITOT TUBE	AXIAL VELOCITY -FIVE HOLE PHOBE
QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	CO, CO ₂ , O ₂ , O ₃ , O		No. Do. Chi. Sanp'e ind Probe and Probe and Chromato Graphy
QUANT	TEMPERA- Ture	THERMO- COUPLE	очет. Солет	тнеямо- соирте
	OF CASES	FOUR DIFFERENT AND TIVE VARYING AMOUNTS OF NY ANDED TO FUEL STREAM.	ONE	ONE
Ē	LOEL	GI4 - AIR	GIY GASAB H2 + CO H2 + CO H3 + CB4 + OTHER GHY)	CH4 - AIR
ě	TYPE	2.0 Parabolic	2-D Parabolic	2-D Parabolic
FLOW DESCRIPTION		VERTICAL FREE JET CH ₄ FLAME IN AIR.	ENCLOSED JEF FLAMEIN A COFLOWING HIGH TEMPERATURE AR STREAM HEATED AIR THE FUEL	CENTRAL FUEL, JET SUSROUNDED BY AIR THROUGH ANHULAR SWIRLER IN A CONICAL COMBUSTOR AIR FUEL
AIITHUR	(VFAR)	HASSAN, LOCKWOOD AND MONEIB (1980) REF. 133 SECTION 6.13	TAKENO AND KOTANF 11975) REF. 134	PAAUW REF, 135

TURBULENT DIFFUSION FLAMES.

TABLE 11.

`		REMARKS	EFFECTS OF LOW REYNOUS MUNBER WFLUENCE OF BUCHNOCY ON THIBBUELING: AND SOOTING EFFECTS POSE SOOTING EFFECTS POSE SONE UNCERTANTY IN ESTIMATING INITIAL CONGENOS: SO CALCULATION CAN BE STARTED FROM FRIST MEASURED LOCATION		ABSENCE OF COMPOSITION MEASURE. ACOUNTS PRECI VOLOGES DRECT VALIDATION OF CREMSTRY MODEL
į	NTIONS	ОТНЕЯ	AXIAL AXIAL REGITY — RADAL PROFILES AXIAL LICATIONS AXIAL VARIATION OF FLUX	AXAL VELOCITY TRANSVERSE PROFILE AT 7 AXIAL LOCATIONS	TP, AXIAL VELODIY VELODIY VELODIY PROFILES AI 24 AI 24 LOCATIONS
. (0	MEASUREMENT LOCATIONS	COMPOSI- TION	RADAL PROFIES A J SARAL LOCATONS	TRANSVERSE PROFILE AT 7 AXIAL LOGATIONS.	
(CONTD)	MEAS	TEMPERA- Ture	RADAL PROFILES AT 3 AVIA LOCATORS		PADIAL PROFIES PROFIES PAZAL COCATIONS
FLAMES	ED AND Inique	ОТНЕВ	AXM. VELOGIY ~ LOY RAUMAINE HEAF FLUX	AXIAL VELOGITY PITOT TUBE	VELOGIY VELOGIY
- 1	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	CH4, H2, CD2: CD1, H2, CD2: N2, N3 SORVIETIC SAMPLING AND GAS CHROMATOS- RAPHY	Cyle, CO. Cys, Oz. Hz. Ny. Saweling Probe. And Probe. And Chromatog. Raphy	
DIFFUSION	QUAN	TEMPERA-	THERIMO- COUPLE		ТИЕВИО- COUPLE
1	NUMBER Of Cases		2 WITH DFFERENT FUEL FLOW RATES	S WITH DOFFERENT INLET VELOCITIES	ONE NON- SYNFLING AND THREE SYNFLING WITH WARYING SWIRL NUMBER.
TURBULENT	FEE		CH ₄ AIR	C3Hg-AIR	CH4-AIR
	FLOW	TYPE	2.D Parabolic	2.0 Parabolic	2-D Parabolic Svarling Swrling Swrling
TABLE	FLOW DESCRIPTION		BUDOYANI AXISYAMETRIC FLAME RISING VERFICALLY IN STAL AR	CONFINED FLAME STABILIZED DNA CYLINDRICAL FLAME HOLIDER IN A RECTANGULAR DUGT FLAME HOLIDER FUSEL & AN FR	ENCLOSED JET FLAME
	AUTROR	(tran)	YOU AND FAETH (1962) REF. 136	SHIPMAN AND CO. WORKERS (1963 AND 1967) REF. 137 REF. 138 SECTION 6.12	HELLAT. LENZ. AMD GUNTHER. REF. 139

		REMARKS	DISCUSSION ON THE ACHIGACY OF MASURE. NENTS PROVIDED COMPUTATIONS WITH AC MODEL REPORTED. PRASONNIRE ACREEMENT WITH DATA.	DISCUSSION ON THE ACCURACY OF REASINGHENIS PROVINCED	DSCUSSON ON THE ACCHARGE RENEWRIES PROYOCD ASSENCE OF TEMPERSONE COMPOSITION MESSINE MENTS PRECTUGES DRECT VALIDATION OF COMBUSTION MODEL
	TIONS	ОТНЕЯ			AXUL VELOCIY, VELOCIY, ILENGE IENGE AXUA PROFILES ALDING CKNTERLINE AND OFF-
	MEASUREMENT LOCATIONS	NOIL LION	RADAL PROFIES AT 8 AXIAL LOCATIONS	RADAL PROFILES AT 7 AXIAL LOCATIONS	
(CONTD).	MEASI	TEMPERA. Ture	RADUL PROFILES A'S AXAL LOCATIONS		
	ED AND NIQUE	OTHER			AXIAL VELOCITY, TUBBUT LENSITY - LDV
N FLAMES	OUAHTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- Tion	D2, N2, H2, CH2, CH2, CH2, CH2, CH2, CH2, CH2	92, 03, 03, 84, 03, 03, 03, 03, 03, 03, 03, 03, 03, 03	
DIFFUSION	QUAKIT NEASI	TEMPERA- Ture	COUPLE -	·	
	NUMBER OF CASES		28 16515	COLD AND HOT FLGW	COLD AND HOT FLOW FOR A COP FERENT COZ AND CQ HIES RAIES
TURBULENT	FUE.		Ctq - AIR	Gtų - AIR	C3.18 - AR CO2 - AR FER COLD FLOW.
11. T	200	TYPE	2.0 ELLPTIC	2.0 ELLIPTIC	2.0 ELLIPTIC
TABLE 1	FLOW DESCRIPTION		AXISYAMETRIC COMBISSIOR WITH COAXIAL FUEL. JAO ARI JEIS A IR F VIEL.	RAMJET DUSAP COMBUSTOR	APL RESEARCH COMBUSTOR: DUCITED BLUFF BOOY COMBUSTOR CONSISTING OF COAXIAL FUEL AND AIR JETS AIR
	AUTHOR	(YEAR)	LEWIS AND SMOOT (1981) REF. 140 REF. 141 SECTION 7.10	CHANG AND TERNAN (1982) REF 124	LIGHTMAN ET. AL. (1980) REF. 142

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	REMARKS	MEASUREMENTS ONLY A! ESTAUNS! THANK— NICOMPLETE ON DETALED VALIONTON		TEMPERATURE AND COMPOSITION MEASURE. MENTS NOT AVNA ABLE DIRECT VALIDATION OF	COMBSSTAN MOCEL NOT Possible	RADATON EFFECTS SAIO TO BE SALVIL L'ANTED ANOUNT OF DATA — L'ANTED UTALITY	
THOMS	OTHER			AXM. VELOGIT - RADIAL PROFILES AT	4 AXIA LOCATRONS, ALSO AXIA PROFILE OF AXIA VELOCITY VELOCITY VELOCITY CENTERINE.	FLAME LENGTH AT 4 SWRL NUMBERS	
MEASUREMENT LOCATIONS	COMPOSI- TION	RADIAL PROFILE AT EXHAUST				CANTOUR PLOTS	
MEAS	TEMPERA- Ture	RADAL PROFILE AT EXHAUST					
ED AND INIQUE	ОТИЕВ	·		L LDV VELOGIY NXIAL		FLAME	
QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	C,H,, CO. EKHAUST GAS ANALYSIS SYSTEM.				AUXTURE FRACTOON: WATEH-COOLED PROBE, GAS ANALYSIS.	
QUANT	TEMPERA- Ture	THERINO- COUPLE					
G	OF CASES	COLD AND HOT FLOSY		COLD AND HOT FLOW		ONE NON: SWIRLING AND FOUR DIFFERENT SWIRL NUMBERS.	
1	1961	CH4-AIR		C3H8-AIR AND C8H18-AIR		CH4-AIR (TOWN GAS)	
à	TYPE	2-0-61.11.11.16		2-D ELLIPTIG		2-DELLIPTIC SWALING AND NON- SWIRLING	
FLOW DESCRIPTION		OPPOSEO JET COMBUSTOR	AIR+FUEL JET TUBE	DILUTE SWIRL COMBUSTOR	SWIRL AIR FUEL CONE/ANNULAR NOZZLE	CYLINDRICAL FURNACE, AXIALLY FIRED BY COAXIAL FUEL And ari jets,	A AIR
AUTHOR	(YEAR)	PECK AND SAMUELSEN !1977) REF. 143		BRUM AND SANUELSEN (1982) REF. 144	SECTION 8.4	EL-MAHALLAWY, LOCKWOOD AND SPALDING REF, 145	

TURBULENT DIFFUSION FLAMES (CONTD).

TABLE 11.

	,	REMARKS	DISCUSSIONS ON THE AC CURACY OF MEASURE MENTS PROFIDED CONSIDERABLE AMOUNT OF DATA FOR DETAILED VALIGATION OF COMBUSTION MODEL.	TEMPERATURE AND COM- POSTION NEXASTERENTS NOT AVALABLE — DIFECT ASSESSMENT OF COMBAS. TON MODEL NOT POSSBLE
	TIONS	OTHER		RADAL FRO- FRES OF U.V. WARD K.A. 6-XXAL LOCATONS
	MEASUREMENT LOCATIONS	COMPOSI- TION	AXM, PRO- FILES AT 2 PADDAL LICOLIDAS. PROJAL PROJAL 2 AXM, LICOLIDAS.	
(CONTD)	MEASI	TEP'YERA- TÜRE	AVIA PRO- FALES AT 2 RADAL LOCA- RADAL LOCA- ROOT ES AT 3 AVIAL LOCATONS	
FLAMES (O AND NIQUE	OTNER		3.7ELOCITY COMPONENTS AND KE OF TURBULENCE. LID
	OVANTITIES MEASURED AND MEASUREMENT TECHNIQUE	: HPOSI- TION	H-Q. Q. N. CQ. CQ. CQ. CQ. CQ. CQ. CQ. CQ. CQ. CQ	
DIFFUSION	QUAIIT Measi	TEMPERA- Ture	THERMO- COUPLE	
	RUMBER OF CASES		3 WITH DIF- FERENT WLE! TEMPERATURE AND EUNIA- LENCE RATIO.	FLOW
TURBULENT			C ₃ Hg-Alf	GRS/AIR GRS/AIR
11.	FLOW	TYPE	20ELIPIG	SWIRLING SWIRLING
TABLE	FLOW DESCRIPTION		OPPOSED REACHING JET COMBUSTOR PREMIXED CANGIANS STREAM STABLISED BY A COONTERFLOWING JET OF THE SAME REACTANTS AND THE SAME REACTANTS AND THE FUEL JET TUBE	CYLINDHICAL COMBUSTION WITH MAUBAL GAS THRUA SLOTS AND THRU AM AXAL INLET PPE. ANGLE ANGL
	AUTHOR (*. AR)		SCHEFER AND SAWYER (1976) REF. 146 SECTION 7.9	CHKJER AND DVORAK (1975) REF. 147

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•		REMARKS	DAIA PROVICED FOR AS- SESSAIRNIT OF COMBUSTION MODEL UNDER SYNELING FLOW CONDITIONS.	EFFECT OF PREIEATING STUDIED. TOSETHER WITH THOURSON, CROCKER AND UNKOUT, THS PROVICES A DETALED DUTA SET.	USED 10 STUDY SWARL EFFECTS UNDCR FEACTING COMPOSITIONS COMPOSITION AND TEMPERA- THER MEACHER SWATE ANALABLE, DIRECT ASSESSA NENT OF COMBUSTION MOGEL NOT POSSIBLE
	TIOMS	OTHER	RADAL PROFIES OF AXIAL VELO- CITY AT 2 AXIAL LOCATIONS.		RUDH PROFIES OF AXIA AND INVENTING VICTORIES AT 3 AXIA LOCKTONS
	MEASUREMENT LOCATIONS	COMPOSI- TION	RADAL PROFIES AT 7 XXVI. LOCATONS	RADAL PRO- RLE AI EXI PLANE AND ONE MORE PROFILE ALONG CENTERLINE.	(A)
(CONTD)	WEAS	TEMPERA- Ture	RADAL PROFIES AT 7 AYAL LOCATORS	CONTOUR PLOT OF WHOLE TELL PERATURE FRELD.	
FLAMES	ED AND INJOUE	ОТИЕВ	- LDV VZAL		AXIAL AND TANGENTAL VELOGITY CUMPONENTS - LDV
	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	CO2, O2, CO. 15, CUAITZ MICHOPROSE AND GAS CHROLAND GRAPHY	CO2, H2, O2, CO, OUANT CANDER MICHOFROBE CHROMATO GRAPHY.	
DIFFUSION	QUANT	TEMPERA- Ture	COUPLE COUPLE	COUPLE:	
	NUMBER Of Cases		3FLANES WITH DIF- FERENT FUBLZ AIR BATTO	A DUFFERNI MLT: AM 7541 PERATURES	TWO — DIFFRENT AMOUNTS OF SWIRL.
TURBULENT			C ₃ Hg·AIR	C ₃ Hg-AJR	GAS-AIR GAS-AIR
11.	FLOW	TYPE	2-DELIPTIC Smrling	2-deliptic Swirling	2 DELLIPIC Swireing Non-Swireing
TABLE	FLOW DESCRIPTION		MASA CONTRA SYRIL CAN TWO COUNTER-ROTATING AMULAR ARRAND ARR FINEL STREAMS IN UNCONFINED STAGMANT ARR. COUNTER-ROTATING ANR ANR FUEL & AIR	NASA CONTRA SWIRL CAN TWO COUNTER-ROTATING ANKULAR AR AND ARR FIJEL STREAMS IN UNCONFINED STAGNANT AIR. COUNTER-ROTATING SWIRLERS AIR FUEL & AIR	CONFINED TURBULENT D'R FUSON FLAME BURNER, CENTRAL FUEL LET AND A COAXIAL ANITULAR AIR STREAM. THE LET AND A COAXIAL ANITULAR AIR STREAM. FUEL LET AND A COAXIAL ANITULAR AIR STREAM.
	AUTHOR	(YEAR)	THOMPSON CHIGER AND UNCUT (1977) REF. 148	THOMPSON, CHICLER AND VENTURA (1978) REF. 149	OWEN (1976) REF. 153

DATA PROYDES FOR MODEL ASSESSMENT INDER SWRG. ING FLOW CONDITIONS. DISCUSSION ON THE AC-CURACY OF MEASUREMENTS PROVIDED. DATA PROVIDES FOR MODEL ASSESSMENT UNDER CON-DITION CLOSE TO THOSE IN GAS-TURBINE COMBUSTORS DATA PROYDES FOR MODEL ASSESSMENT UNDER COMO-TIONS CLOSE TO THOSE IN GAS TURBINE COMBUSTORS FLOW SPLITS THROUGH PRIMARY JETS NOT GIVEN, CAN BE CALCULATED BY ANNILUS LOSS MODEL. REMARKS CONTOUR PLOT OF AXIAL AND TANGENTIAL VELOCITIES OVER COM-PLETE FIELD. COLD FLOW LU, WAT 3 LU, WAT 3 CROSS-STREAM PLANES. HOT FLOW LU, Y. AT Z AXUA. AUD 4 CROSS-STREAM PLANES. **CTAER** REASUREMENT LOCATIONS CONTOUR PLOT OF COM-PLETE FIELD AS FOR TEMPERATURE COMPOSI-TION COLD FLOW: 3 AXIAL AND 3 CROSS-STREAM FLANES. HOT-FLOW: 4 CROSS-STREAM AND 3 AXIAL PLANES. (CONTD). CONTOUR PLOT OF COM-PLETE FIELD. HOT FLOW: 4 CROSS-STREAM AND 3 AXIAL PLANES UPSTREAM
OF FURATY
JETS, END OF
PRIMATY
ZONE, 3
INTERMETATE
PLANES AND
JUST UP
STREAM OF
DRUTTON
JETS. TEMPERA Ture AXIAL AND
TANGENTIAL
VELOCITY
COMPONENTS
— LDV.
STREAMLINE
PATTERN. COLD FLOW: U.V.W. - LDV. HOT FLOW: U.V. - LDV. OTHER OVANTITIES MEASURED AND MEASUREMENT TECHNIQUE CO, C3HB, H2.
EQUIVALENCE
RATIO SAMP.
LING PROBE
AND GAS
ANALYSIS. COMPOSI-Tion CH4.CO TEMPERA-Ture THERMO. THERMO-COUPLE THENMO-COUPLE COLD AND HOT FLOW, 2 FLUW CONDITIONS EACH. NUMBER OF CASES COLD AND Hot flow 뽕 뎚 CH4-AIR NATURAL Gas-air C₃Hg-AIR 2-D ELLIPTIC SWIRLING 3-DELLIPTIC 3-DELLIPTIC FLOW RESEARCH CAN COMBUSTOR; SIMPLIFIED GEOMETRY INCORPORATING THE MAJOR FEATURES OF GAS-TURBINE COMBUSTORS. FLOW DESCRIPTION Variable Area Primary Ports Dilution Forts COAXIAL FUEL AND AIR SWIRLING JETS. SECTOR OF AN ANNULAR COMBUSTOR. , THE CLAYPOLE AND SYRED (1981) AUTHOR (YEAR) REF. 151 NOYCE SHEPPAND AND YAMBA-(1981) TORAL (1980); Toral And Whitelaw (1982) REF. 152 REF. 153 REF. 154

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TURBULENT DIFFUSION FLAMES

TABLE 11.

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		REMEMBO	DECUSSION ON ACCUBACT OF MEASUREMENTS PROVIDED. ALL DIMENSIONS AND FLOW SPILIS NOT CHERT HITSER- SPILIS NOT CHERT HITSER MEGESSARY FOR MODELING.
	TIOKS	OTHER	RADAL PRO- FILES OF AXIAL (TOCATIONS)
•	MEASUREMENT LOGATIONS	COMPOSI- TION	RADAL PROFILES AT 7 AXIAL LOCATIONS.
(CONTD).	MEAS	TEMPERA- Ture	RADAL PROFILES AT 7.A.Y.L LOCIONS.
FLAMES (ED AND INIQUE	ОТНЕВ	VELOCITY: 7 HOLE PRIOT PROBE
- 1	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	02, N2, O3, O3, O3, O3, O3, O3, O3, O3, O3, O3
DIFFUSION	OUANT MERS	TEMPERA- Tuke	обирт. Е
- 1		NUMBER OF CASES	
TURBULENT			G3ttg-AIR
11. T		TYPE	3-E ELLIPTIG
TABLE 1	FLOW DESCRIPTION		Switer Air Dilutior Cooling Air Igniers Cooling Air Property Prope
	AUTHOR (YEAR)		1977) HEF, 155

5.1.3 Spray Evaporation and Combustion

In this paragraph, a data base for assessing spray evaporation and combustion models is provided. The assessment procedure will consist of comparing the predicted spray trajectory, droplet concentrations, velocities and size distribution, temperature, and concentrations of species (unburnt fuel, CO, CO₂ H₂, H₂O, O₂, N₂) against the experimentally measured values of these quantities. The available data on spray evaporation and combustion is listed in Table 12. The predictions of these quantities is an indication of the accuracy of the various features of the spray model:

- The prediction of spray trajectory, droplet concentrations, velocities, and size distribution under nonburning and nonevaporating conditions reflects on the accuracy of the spray dynamics model, which includes the modeling of the drag forces between the spray and the gas phase.
- O The prediction of the droplet concentrations and size distributions along with the mixture fraction under non-burning (but evaporating) conditions serves to test the droplet heat-up and evaporation models.
- o Finally, the prediction of droplet concentration and size distribution along with gas temperature and composition serves to test the validity of the spray combustion model.

Thus by assessing the predictions of the quantities listed above, all features of spray evaporation and combustion involving interphase momentum (spray dynamics, drag), reat (droplet heat-up) and mass (droplet evaporation and combustion) transfer are tested individually and jointly.

ity. Sources in which all boundary and initial conditions required for modeling were not completely or clearly stated have not been included in the data base (e.g. References 156-170). It should be noted that complex two-phase slip models as used at Garrett require detailed information specifying the initial conditions at the fuel injector; initial drop size distribution, initial velocity distribution, etc. This information is generally not available and therefore has to be estimated from the available injector characteristics.

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	REMARKS	SINCE MEASUREMENTS WITH AND WYD SPARY WIDGEN HOT AND CULD COMONIONS ARE AVALABLE A SYSTEMATIC STEPWISE TESTING OF THE MODEL IS POSSIBLE	TEMPERATURE MEASURE MENTS OUALITATIVE, SINCE DROP IMPINEMENT EF- FEUTS KNOMED. LOCALLY HOMOGENCOUS FLOW PREDICTIONS OFFER ESTIMATE RAIT OF FLOW BOYELCOMENT BY 20-40%, SYSTEMATOR STEPWISE NALIOMATION YOSSSBLE WITH THE THREE CASES.	LOCALLY HOMOGENEOUS FLOW PERCEITOMS OVER ESTIMATE FAITE OF FLOW EVELOWMENT BY ~ 30%, GOOD GAREARIN OF PRE- DICTIONS WITH DAIL OF PRE- PROPAUR FLAME WITH THEN TOCETHER WITH THIS TOCETHER WITH
w w	ОТНЕЯ	RADIAL PROFILES OF GAS VELOCITY AG AVIAL LOCK HONS	RADAL, PROFILES OF GAS VELOCITY AND TURE NITENSITY AT 3 AXIAL LOCATIONS ALSO AXIAL PROFILES CENTER- LINE	RAGAL PHOFILES OF GAS VELOCITY AND TUB- BULENCE WINENSITY AVAIL LOCA- TIONS AXIAL AXIAL AXIAL ALONG CENTER- LINE
MEASUREMENT LOCATIONS	COMPOSI- TION		RADIAL PROFILES AT 3 AXIAL LOCATIONS: ALOCATIONS: PROFILE ALONG CEN TERLINE.	RAGIAL PROFILES AT 4 AXIAL LOCATIONS
EASUREMEN	TEMPERA- Ture		RADIAL, PROFILES AT 2 AXIAL LOCATONIS, PROFILE ALONG CEN TERLINE	RADIAL PROFILE N 4 AXIAL LO- CATIONS. AXIAL PRO- FILE ALONG CENTER- LINE
	SPRAY	DROPLET CONCEN- IRATION - RUDAL - RUDAL A SAVIAL LOCA- IONS, DROPLET SIZE AND VELOCITY - RADAL PROFILES AT 6 AXIAL	DROP SMD MEASURED AT THREE AXAL AND THREE ROBAL LOCATIONS (9 LOCA- TIONS)	
, 全 型	OTHER	GAS VELO- CITY LASER TOMO- GRAPHY	GAS VELO- CITY AND TURBU- LENCE INTENSITY - LDV	GAS VELO- GIY AND TURBU- TENGEN- TENGEN- LOV
IEASURED AN IT TECHNIQU	COMPOSI- TION		MIXTURE FRACTION - ISO- KINETIC SAMELING AND GAL AND GAL CHEDIAA- TOGRAPHY	CO. Ca16. Na. Oz. CO. Hy. Ho. – Hy. Ho. – SAWITING AND GAS CHROMA TOGRAPHY
QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	TEMPERA. Ture		COUPLE COUPLE	оличе Оличе
	SPRAY FEATURES	DROPLET VOLUME CONCEN- TRATION: DROPLET VELOGITY: USING LASER TAN	DROP SIZE DISTRIBU- TON AND LIOURD ASS FLUX - SLIDE IMPACTION	
5	OF CASES	FOUR: TWO WITH SPRAY (HOT & COLD) TWO W/O SPRAY (HOT & COLD) HOT = EVAPOR- EVAPOR- COLD = NON-EVAR- ORATING	THREE: 1)1SO- THEBIAL AR JET 2)1SO- THERMAL DENSE GAS JET 3) EVA PORATING SPRAY JET	ONE WITH EACH FUEL.
9	<u> </u>	KEROSENE	FREON-11	GASEOUS PROPANE: LIQUID N-PENTANE
ac	TYPE	2-0 Parabolic	2-0 Parabolic	2-D PARABOLIC
FLOW DESCRIPTION		UIHBULENT KEROSENE SPRAY INJECTED INTO A COFLOWING AIR STREAM THROUGH A TWIN FLUID ATOMIZER. IN JECTOR SPRAY	JET ISSUING VERTICALLY DOWNWARD INTO STABMANT AIR. IN JECTOR JOHN SPRAY	JET ISSUING VERTICALLY UPWARD INTO STAGNAMI AIR, AIR ATOMIZED SPRAY. SPRAY
AUTHOR (YEAR)		YULE ET AL. (1962) Ref. 171	SHEARER AND FRETH (1979) REF. 172	MAD, SZEKELY AND FAETH (1980) REF. 173

SPRAY EVAPORATION AND COMBUSTION.

TABLE 12.

		······································	> >			·
		REMARKS	COMPARSON BETWER GASEOUS AND SPRAY FLAMES FOR SARL AR COMMIND POSSUE E— HELPS IN ASSESSING SPRAY AND GASEOUS COMPISTION MODELS.	DETALEDDATA SET FOR MODEL ASSESSMENT UNDER DUFFERNT FLOW SON-DITONS.	SOME GEOMETRICAL DE: TALS NOT EXRETLY KNOWN	SOME PROBLEMS POSED IN MODELINGS GOOD FUEL IMPINESKEIN ON INWER TUBE WALLS.
	బ	OTHER	AXIAL PROFILE OF GAS VELOCITY ALONG CENTER- LINE, HADAL PROFILE AT ONE AXIAL	CONTOUR PLOT OF GAS VF- LOCATY	RADAL PROFILES OF GAS VELOCITY AT 8 AXIAL LOCA- TONS.	
2	NT LOCATION	COMPOSI- TION	AXIAL PRO- FILE ALONG CENTER- LINE. FADAL PROFILE AT ONE AXIAL LOCATION.	CONTOUR	PLOTS PLOTS	CONTOUR
(COMPD.)	MEASUREMENT LOCATIONS	TEMPERA- Ture	AXIAL PRO- FILE ALONG CENTER- LINE LINE RADAL PROFILE A AXIAL LOCATION.	CONTOUR PLOTS	RADIAL PROFILES AT BAXIAL LOCATIONS, CONTOJIR PLOTS.	PLOTS
		SPRAY FEATURES	HADAL PROFILE OF DROP- LETNO DENSITY AT 3 AXIAL LOCK- TOWN.S. DROPLET SIZE DIS- TRIBUTION AT 4 LOCK- TOWN.S.	CONTOUR PLOT OF DHOPLET VELOCITY.	VAPORI- Zation Region.	
COMBUSTION		OTHER	GAS VELOCITY - PIOI TUBE.	GAS VELOCITY - LDV	GAS	
	QUANTITIES MEASURED AND Measurement technique	COMPOSI- TION	O. CO. CO. C.H. C.H. SOOLEB SAMEING PROBE AND GAS CHROMA- TOCRAPHY	CO,	CO2 CO, O2: SAMPLING PROBE AND GRAS GRANA TOGRAPHY AND IN- FRARED ANA	G, H, CO. CO, G, COOKED COOKED SAMPLING PROBE AND GAS AMAIYSIS
ON AND	DUANTITIES MEASUREME	TEMPERA- Ture	THERMO- COUPLE	THERING- COUPLE	THERMO. COUPLE	COMPOSI- TOM, KG- TOM, KG- MORING PRESENCE OF H2. INERMO- COUPLE
RATIC		SPRAY FEATURES	DROPLET NO. DENS- ITY AND SIZE — CLASS RATE COL- LEGIOR AND MI- CROPHOTO- GRAPHS.	DROPLET VELOCITY - LDV. DROP SIZE AND SPRAY TRALEGT- ORY - LASER HOLO- GRAPHY.	EXTENT OF DROP VAPORIZA- TON USING INDICATION DYE.	
EVAPORATION	Nith	OF CASES	THREE FOUL VALENCE RATIOS FOR LIQUID FUEL; ONE FORGAS- EGUS FUEL; AND ONE ISO- THEMAL LIQUID FUEL.	TWO SWIRL ANGLES: TWO PRES: SURES; TWO INLET TEMPERA- TURES.	THREE JET TO AN VELOCITY NATIOS.	ONE FOR EACH FUEL.
SPRAY I	폂		CASEOUS PROPANE AND LOUID KENDSENE	ISO. OCIANE AND H2 DISTILLATE FUEL OIL	KEROSENE -	LIQUID PROPANE AND JETA
SP	FLOW	TYPE	2-0 ELLIPTIG	2-0 ELLIPTIC	2.D ELLIPTIC	2.0 ELIPTIC
TABLE 12.	FLOW DESCRIPTION		CYLINDRICAL BURNER WITH ANA MR.ATOMIZING SPRAY NOZZLE AND ARI RITRODUCEO THROUGH AN ANNULUS SUR- ROUNDING THE NOZZLE A17	CYLUNDRICAL COMBUSTOR WITH CENTRALY LOCATED PRESSURE ATOMIZING FUEL INJECTOR, AIR MITRODUCED THROUGH AN ANNULUS SWIRLER AROUND FUEL "AJECTOR. ALE AND ANNULUS SWIRLER AROUND FUEL "AJECTOR. ALE AND ANNULUS SWIRLER AROUND FUEL "AJECTOR.	·····	PREVATORIZING/PREMIXING COMBUSTOR SHROUDED TUBE AND DISC CONFIGURATION, SIMPLEX PRESSURE ATOMIZING NOZZLE. COMBUSTOR SHROUD COMBUSTOR SHROUD TUBE
	AUTHOR		ONUMA AND OGASAWARA (1975) REF. 174	SPADACOM ET AL. (1977) REF. 175	WIERZBA (1982) Ref. 176	PROCTOR AND MELLOR (1982) REF. 177
			,			

DROPLET SIZE DESTRBUTION AND INJECTION VELOCITY MEASURED — INLET CONDITIONS ACCURATELY KNOWN. SOME PHOBLEMS POSED IN MODELING LIQUID FUEL IMPINGEMENT ON INNER TUBE WALLS. ASSESSMENT OF MEASURE. MENT ACCURACY PROVIDED REMARKS RADIAL PROFILE OF AXIAL VELOCITY AT 3 AXIAL LOCATIONS. **REASUREMENT LOCATIONS** COMPOSI-TION RADIAL PROFILES AT 8 AXIAL LOCATIONS. CONTOUR PLOTS OF CO AND C₂H₃, CONTOUR PLOTS TERPERA-Ture RADIAL PROFILES AT B AXIAL LOCATIONS. CONTOUR PLOTS. SPRAY FEATURES PROBLE
OF AXIAL
VELOCITY
AT A AXIAL
LOCATIONS
AND OF
TIANGENTIAN OTHER ISO-THERMAL AXIAL VELOCITY QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE CO – SAMPLING PROBE; NON-DIS-PERSIVE INFRARED ANALYZER; CAH, — FLAME CONIZATION DETECTOR. COMPOSI-TION SAMPLING PROBE, INFRARED ANALYZER, 02 – PARAMAG-NETIC ANA-LYZER, CO2, CO — SAMPLING PROBE, IN-FRARED ANALYZER, O2 — PARAMAG-NETIC ANALYZER, TEMPERA-Ture THERMO: COUPLE WALL TEMP: ERATURE MEASURED. THERMO-COUPLE THERMO. COUPLE SPRAY FEATURES AXIAL AND TANGEN-TIAL DROP-LET VE-LOCITY – LOY KUMBER OF CASES SIX WITH DIFFERENT SIAD AND AIR SWIRL ISO-THERIKAL AND COM-BUSTING 뽏 KEROSENE KEROSENE FUEL JET-A 2:D ELLIPTIC FLOW 2.0 Elliptic 2.D Ellptic COMBUSTOR PREVAPORIZING/PREAIXING COMBUSTOR-TUBE AND DISC Configuration; Simplex pressure atomizing nozzle, CYLINDRICAL COMBUSTOR WITH ROTATING CUP ATOMIZER AND AIR THROUGH A SWIRLER SURROUNDING ATOMIZER. - DISC FLOW DESCRIPTION AS EL-BANHAWY AND WHITELAW (1979) FUEL TUBE -FUEL FIFUEL Å AIR EL-BANHAWY & WHITELAW (1981) EL-BANHAWY & WHITELAW (1979) SECTION 8.7 AUTHOR (YEAR) FERGUSON AND MELLOR (1979) REF. 178 REF. 179 REF. 180

(CONTD).

SPRAY EVAPORATION AND COMBUSTION

12.

TABLE

		REMARKS	ASSESSMENT OF MEASURE. MENT ACCURACY PHOVIDED	UMITED AUGUAT OF DATA FOR DETAILED MODEL ASSESSMENT.	DROPLET SZE AND VE. LUCITY DATA PROVIDE FOR ASSESSIENT OF SPRAY WODEL FFATURES.
	83	OTHER	RADIAL PROFILES OF GAS VELUCITY AT 5 AXIAL LOGA- TIONIS.		CONTOUR P. COLS OF AXIAL VELOGITY
(CONTD).	MEASUREMENT LOCATIONS	COMPOSI- TION	AXIAL ALONG GENIER- LINE. RADAL PROFILE AT 3 AXIAL LOCATIONS.	RADAL PROFILES AT 5 AXIAL LOCATIONS	RADIAL PROFILES PROFILES LOCATIONS AXIAL PRO- THE ALONG CENTER- LINE
	MEASUREME	TEMPERA- Ture	AXIAL FIRGUE E CENTER. CENTER. LINE. BADAL PROFILE AT 3 AXIAL LOCATIONS	RADIAL PROFILES ATS AXIAL LOCATIONS	RADIAL A PROFILES A PROFILES LOCATIONS. AXIAL PRO- AXIAL PRO- TILE ALONG CENTER- LINE.
STION		SPRAY FEATURES	RADAL PHOLITE OF DHOL LEI NO DEHSITY AI 4 AXIAL LOCA. HOCA.		PRODAL PROFILES OF DROPS- LET SIZE AND VE- LOCITY AT 2 AXIAL LOCA- TIOCA
COMBUSTION		ОТНЕВ	GAS VIOGIY IIN	·	AXIAL VELOCITY LDV
AND C	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	00.002 – COOLED SAMPLING PROBE. INFRARED ANALYZER, OZ – PARAMAG. RETIC GHL, — FLAMEON- ZATION DETECTOR.	4.7.00 14.7.00	CO. CO2- H2. CH4 QUARTZ MICRO- PROBE AND GAS CHROMA- TOGRAPHY
	DVANTITIES NEASUREME	TEMPERA- Ture	COUPLE	THERMO- COUPLE	тневио.
EVAPORATION		SPRAY FEATURES	DROPLET NUMBER DENSITY - LDV.		DROPLET SIZE AND VELOCITY VELOCITY DIFFAC. 100 TECH- NIQUE AND LASER ANEAR METER
	NUMBER Of Cases		TWO DIF- FERENT SMD'S.	ONE	HOT AND COLD FLOW.
SPRAY	Fee		KEROSENE	LICKID PROPANE	KEROSENE
12.	FŁOW	TYPE	2-0 El LIPTIG	2.0 ELLIPTIC	2.0 ELLIPTIC
TABLE	FLOW DESCRIPTION		VERTICAL SPRAY FLAME IN STILL ARE STABILIZED ON A DISC AF DEL MOZZIE ENT PLANE, SOI ID COME SPRAY WITH 1 WIN FLUID ALOMATER SPRAY STABILIZING STABILIZING STABILIZING STABILIZING	SIMPLEX PRESSURE ATOMIZER AIR	TWIN FLUID ATOMIZER UNCONFINED FLAME STABILIZED IN A COFLOWING AIR STREAM ON A DISC AT ATOMIZER EXIT A TO THE STABILIZED IN A COPE OF THE STA
	AUTHOR		AITYA AND WHIFELAW (118811) REF. 181	TUTILE SHISLER AND MELLOR (1976) REF. 182	STYLES AND CHIGER (1977) REF. 183

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		REMARKS	DATA PROVIDES FOR MODEL ASSECUERT UNDER COMDITIONS ELUS: TURBURE COMBUSTORS.	-
	8	ОТНЕЯ		
(CONTD).	MEASUREMENT LOCATIONS	COMPOS!- TION	RADAL PRO-LES AT 3 AXIAL LOCATIONS.	
	MEASUREME	TEMPERA. Ture	RADIAL PROFILES AT JAXIAL LOCATIONS	
STION		SPRAY Features		
LON AND COMBUSTION	SN SH	OTHER		
	QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	COMPOSI- TION	00 – WATER COOLED PROBE, NOR-DS- PERSIVE INFRARED ANALYZER. G,W, – FLAME KNUZATION DETECTOR.	
	UANTITIES A REASURENE	TERPERA- Ture	THERMO-COUPLE.	
EVAPORATION		SPRAY FEATURES		
	NUMBER OF CASES		4 CASES WITH DIF- FERENT INLET TURES AND DIFFERENT SPLITS.	
SPRAY	F	•	KEROSENE	
12.	FLOW	TYPE	3-0 ELLIPTIC	
TABLE	FLOW DESCRIPTION		CAN COMBUSTOR WITH AIRBLAST ATOMIZER AND AIR INTRO- DUCED THROUGH PRIMARY RADIAL SWIRLER, SECONDARY AND DRUITON HOLES, SECONDARY DILLUTION AIR PRIMARY AIR—EX	,
	AUTHOR	Ewil)	KANWGUCHY EL AL. (1983) REF. 184	

5.1.4 Soot Formation and Oxidation

In this paragraph, a data base for assessing soot formation and oxidation models is provided. The assessment procedure will consist of comparing the predicted soot concentration, temperature, concentrations of species (unburnt fuel, CO, CO $_2$, H $_2$, H $_2$ O, O $_2$, N $_2$) against the experimentally measured values of these quantities. The comparison of predicted and measured soot concentrations is a direct indication of the accuracy of the soot model. Temperature and gas composition are affected by the presence of soot to an extent depending on its concentration. Therefore, assessing the accuracy of the predictions of temperature and gas composition serves to indirectly assess the soot model.

The data base for the soot models is rather inadequate since very few measurements under controlled conditions have been reported in the literature. The reason is the difficulty in accurately measuring soot concentration profiles in a combustor. Quite often, only the exhaust smoke concentration is measured and soot profiles have been measured in only simple flames.

As in the preceding sections, several sources of data (e.g. References 185-194) were found that were not suitable for model assessment due to incomplete specification of the boundary and initial conditions. These have not been included here. Also, measurements related only to gas turbine type fuels have been considered, since it is practically impossible to validate the model and obtain a set of model constants for all types of hydrocarbons. The data base for soot formation and oxidation is presented in Table 13.

THS DATA CAN BE USED TO ESTABLESH RATE COM-STANTS W SOOT FORMA. TRANDATORATOR SINCE UN-CERTARTIES WIR COW AND THRUMA. THRUMA. THS DATA CAN BE 11SED
TO ESTABLESH RATE CONSTANT'S NO SOOT FERBLA.
TOW/OXDATION SINCE UNCERTAMENES IN FLUX AND
TURBULENCE ANE LIBESHT. DATA CAN DE USED FOR ESTABLISHING RATE CONSTANTS IN SOOT FORMATION/OXIDATION REMARKS OTHER **WEASUREMENT LOCATIONS** COMPOSI-TEKPERA ALONG FLAIKE AXIS. SOOT FEATURES SOOT FRACTION FRACTION AND PAR-TICLE SIZE ALCHS FLAME AXIS. SOOT CON-CENTRA-CENTRA-PARTICLE SUZE NI BURNT BURNT BURNT GCAS RE-GCAS RE-GCAS RE-GCAS RE-GCAS RE-GCAS RE-GCAS RA-RULL LO-CATIONS. PANTICLE
DIAMETER,
NUMBER
DENSITY
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VOLUME
FRACTION
ALONG
FLAME
AXTS. OTHER QUANTITIES HIEASURED AND REASUREMENT YECHNIQUE COMPOSI-TEMPERA-TURE THERMO SOOT WALLINE FRACTION AND PAR-TICLE SOFF LICSTR-LICSTR-LICSTR-LICHT SCATTER-RIC AND ABSORP-RIC AND ABSORP-RIC AND ABSORP-RIC AND RIC A SOOT COM-CENTRA-TON AND PARTICLE SIZE -SIZE -SIZE -SIZE -SIZE -SIZE -SIZE -SIZE -NOTE -NOTE -NOTE -PARTICLE
DIAMETER,
PARTICLE
DIAMETER
DENSITY
SOOT
VOLUME
— DIFFUSION
BROAD
B THREE EQUI-EQUI-EQUI-RATIOS; THREE GAS VELOG-THES. NUMBER OF CASES DAFFERENT C/O RATIOS. THREE
DIFFERENT
EQUIVALENCE
RATIOS. FIEL CN 02 AND C3H8 02 C3Hg-72 AND - 54Hg +H2-02 5, € 1-D PARABOLIC 1-D PARABOLIC 1-D PARABOLIC FLOW WATER-COOLED POROUS PLATE FLAT FLAME BURNER, FLAME ENCLOSED IN SKORT CYLINDER PLACED ABOVE BURNER PLATE. FUEL-RICH PREMIXED LAWINAR FLAT FLAME ABOYE A COOLED POROUS-PLUS BURNER. PREMIXED FLAT LAMINAR FLAME STABILIZED RETWEEN A TWIER-COOLED SINTERED BRASS PLATE AND A STAINLESS OSC PLATE ABOVE THE BURNER. FLOW DESCRIPTION AUTHOR (YEAR) BOCKHORN E.T. AL. (1981) Ref. 158 PRADO ET.AL • (1581) REF. 195 FLOWER-(1962) Ref. 197

SOOT DATA.

13,

TABLE

SOOT CONCENTRATION
MEASURED MAY BE IN ER. .
ROM BY A FACTOR OF 1.5-2.0. SOOT PARTICLE SIZE FOUND TO BE ABOUT UNIFORM THROUGHOUT BURNOUT PECSON. CAY, FUE, NOT OF DIRECT INTEREST FOR GAS-TURBINE COMBUSTORS. REMARKS TRANS-VERSE PROFIES OF AXIAL VELOCITY AT 8 HEIGHTS ABOVE BURNER LP. WEASUREMENT LOCATIONS COMPOS TEMPERA-TURE TRAMS.
VERSE
PROFILES
AL 6
HEIGHTS
ALBOYE
BURNER
LP. SOOT FEATURES CONTOURS OF SOOT CONCEN-TRATION RADDAL PHGFLES OF SOOT CONCEN-TRATON AT 10 ASSAL LIDCA-TIONS. TRANS-VERSE PROFILES AI 6 HECHTS ABOVE BURNER 語語 SOOT DATA (CONTD) AXIAL VELGOTY -- LDV. **OUANTITIES MEASURED AND MEASUREMENT TECHNIQUE** COMPOSI-TION TEMPERA THERIMO-COUPLE SOOT SOOT COM-CENTRA-TON --OPTICAL ABSORP-TICN USING A SENSI-TIVE DUAL-BEALL DENSI-TOMETER. SOOT COM-CENTRA-TION -LIGHT SCATTER-RAG SOOT VOLUME PRACTION, PARTICLE MANABER DENSITY AND AVER-ACE PAR-INCLE SZE — LICHT SCATTER-ING SCATTER-ING FOUR VALUES OF EQUIVAL-ENCE RATIO. NUMBER OF CASES 13. 뿕 뿡 TABLE 肥 ਣੱ 22.5 袤 2-0 PAEABOLIC 2-D PARABOLIC FLOW 2-0 PARABOLIC COAXIAL FUEL/AIR JETS -- LAMINAR DIFFUSION FLAME MOOFFED WOLFHARD-PARKER BURNER — LAMINAR OFFUSION FLAME FREE TURBULENT ACETYLENE DIFFUSION FLAME IN STAGNANT AIR FLOW DESCRIPTION Fue, ROPER AND SMITH (1979) REF. 198 AUTHOR (YEAR) DALZELL ET Al. (1970) REF. 199 KENT ET AL. (1981) REF. 200

TABLE 13. SOOT DATA (CONTD).

			2 to	_ ¥
PENABKS		MET VELOCITY AND TEMPERATURE PROFLE MEASURED. FIRE DRUTED WITH N2 AND H-20.	RIDATION MENSYREHENTS PROVICE FOR ASSESSMENT OF NACHTON MODEL ALSO.	CAMPLES FOR UNI OF DIRECT WATERS FOR WAS TO WATER STATES FOR WATER STATES
	OTHER		TOTAL RACK/TON FROM FLAME.	
T LOCATION	COMPOSI- TION			
MEASUREMENT LOCATIONS	TEMPERA		440	
	800T FEATURES	ASSULPSO- PREOF SOUTCON- CENTRA- TOWN ALONG CENTRI- LENE	SALOCE BANSSONS A EXT PLANE,	SOOT COM- CENTRA- TION AUNE FLAME AUS.
24	OTHES		FLAME RADATION - WATER- ENCENTED TO ELENED TO FOLKAL DIOMETER.	
EASURED AS T TECHNIQU	COMPOSI- TYON		,	
QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	TEMPERA. TURE			
82	800T FEATURES	SOOT COM- CENTRA- LIGHT - LIGHT - SIGATTER- RAG METHOD.	SOOT COM- CENTRA- TION - TION - SALFING FATER.	SOOT COM- CENTRA- TION - TION - SCATTER- MG TECH- NOUE.
	NUMBER OF CASES	8 0.955	MEASURE NEATS ON-SYA FRANCE OF AET VE LOCATES LOCATES OD-F METERS.	ONE FOR
į	1	. 4ro	G4. C2.12. C2.14. C2.14. C3.18.	\$ 50 50 50
FLOW		2-0 PARABOLIC	2-0 PARABOLIC	2-0 PARABOUIC
FLOW DESCRIPTION		VERTICAL FREE TURBULENT DIFFUSION FLAME IN STAGNANT FRE	FREE TURBULENT DIFFUSION FLAME. BURNER CCASSISTS OF PAIR OF COAXAL, TURES WITH INNER FUE. STREAM AND AWAULAR STARKZING H _P FLOW (AUST ENOUSH TO SUPPRESS LETOFF). AIR HZ FUEL HZ AIR AIR AIR	AS BECKER AND LUANG (1962) AIR AIR AIR AIR
AUTHOR (YEAR)		MAGNUSSEN ET AL. (1979) REF. 201	BECKER AND LIANG: 4:882) REF. 202	BECKER AND YARAZAKI (1977) REF. 203

TABLE 13. SOOT DATA (CONTD).

HEMARKS		ERROR PROVIER.	DATA PROVICES FOR ASSESSMENT UNCEN DIF- FERENT FLOW CONCUTIONS.	RATE CONSTANTS FOR DIESE, FHEL PROBABLY DIFFERENT FROM THOSE OF MANTON FIELS.	
	OTHER	: 1		,	
T LOCATIONS	COMPOSI- TYN			CONTOUR PLOTS OF CO, CO ₂ :	
MEASUREMENT LOCATIONS	TEMPERA-				
3	\$00T FEATURES	AX3AL PROFALE OF SOOT CONCEN- TRATIONS ALONG CENTER- LINE.	AXAL PROCILE CO-SOOT CO-SOOT CO-SOOT ALONG CENTER- LINE.	CONTOUR PLOT OF SOOT COM- TION	
a	OTHER				
EASURED AN	COMPOSI-			CO, COZ, — COUENCISE STEAM LESS STETE PROBE AND GAS ARATSIS.	
QUANTITIES MEASURED AND MEASUREMENT TECHNIQUE	TENPERA- Tune				
33	SUOT FEATURES	SOOT COM- CENTRA- TICN — WATER COCE ED PROSE AND SALEPLING BLIFEL	SOOT CON- CENTRA- TOW - TOW - TOW - PROSE AND PROSE AND	SOOT CON- CENTRA- TOW TOWN TOWN TOWN STAINLESS	
	AUMBER OF CASES	SVALUES OF EQU- VALENCE AND EAST AND PRES- SURES-2 COLD GAS VELOCI- TIES	FCURICEO- METRRES AND THREE ATOMETSING SURES.	Ove	
i	FUEL	AVATON KEROSENE AND BENZENE	VARIOUS BLENDS OF DIFFERENT FUELS.	DRSEL FUEL	
	TYPE	2-0 ELLPTG	2-0 ELLIPING	2.0 GLIPTIC	
	FLOW DESCRIPTION	CYLINDRICAL BURNER WITY AIR ASSIST FUEL SPRAY NOZZLE AND AR WIRGOUGED THEYUCH SWIRLER SURROUNDING THE NOZZLE.	FLAME TUBE BURNER CONSISTING OF A CROULAR TUBE WITH ACENTRALLY PLACED FUE. INJECTOR SURROUNDED BY AN AIR SWIRLER. AIR SWIRLER. AIR THIS GEOMETRY AND ITS VARIATIONS	CTINUARCAL COMBUSTOR WITH A CENTRAL FUEL IRREGION AND A COLAXIAL ANYOL AR AIR STREAM. AND A COLAXIAL ANYOL AR AIR STREAM. AIR =================================	
AUTHC** (YEAR)		PRADO ET AL.' (1977) REF. 204	HOULT (1979) REF. 205	JANOTA ET AL (1977) REF. 206	

5.2 Data Base from Garrett Gas Turbine Combustors

A number of gas turbine combustors have been mapped at Garrett over the last ten years. A brief description of the Garrett data base is given in the following paragraphs.

5.2.1 Can Combustor Mapping

A nonreacting can combustor with swirlers at the dome was mapped 207 in 1973 for comparison with the k- ϵ turbulence model. A schematic of the burner along with the flow split is shown in Figure 5.2-1. A calibrated three-hole wedge probe and liquid micromanometer were used to measure the radial distirubtion of the yaw angle, static and total pressures at different axial stations.

As part of model validation under the USARTL Design Criteria Program, another can combustor nonreacting flow was mapped at different throughflow rates. This combustor was filled with 21 measurement ports.

A calibrated five-hole pyramid probe was traversed across the can combustor at three circumferential locations and seven axial stations. Four traverses were made in the primary zone, seven in the intermediate, and ten in the dilution zone. The probe mounts and the test conditions are shown in Figure 5.2-2.

Reacting flow mapping was accomplished on a similar can combustor, shown in Figure 5.2-3. Radial profiles of CO, $\rm CO_2$, $\rm NO_x$, and unburned hydrocarbons were measured at axial stations 6.0, 8.5, 10.4, 12.9, 15.4, 18.8, 21.3, and 26.2 cm downstream from the fuel nozzle face. Five circumferential stations were mapped to determine the profile variations in the circumferential direction. The mapping was conducted for both gaseous (natural gas) and liquid fuels (Jet A) over a wide range of operating conditions. The fuel nozzles used for each fuel are shown in Figure 5.2-4.

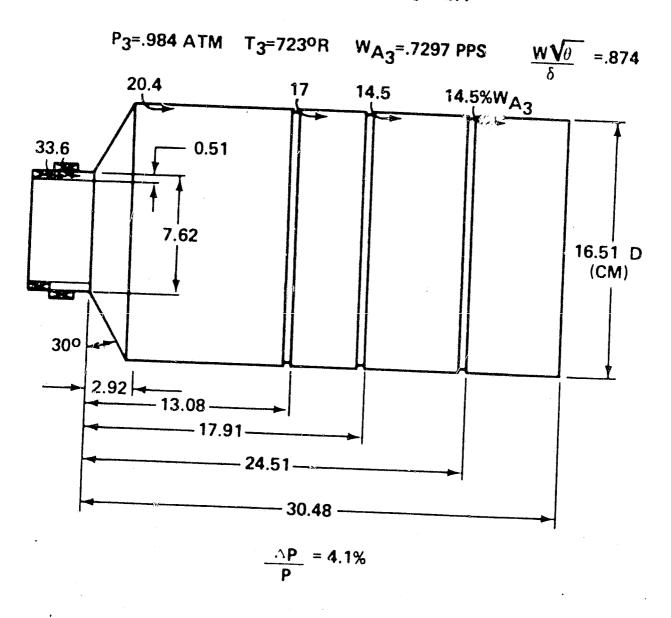
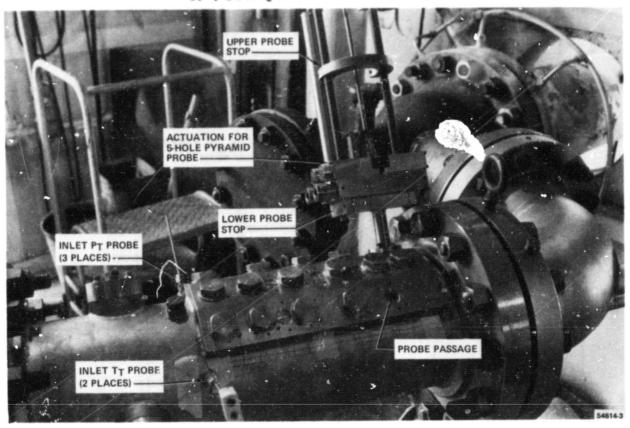


Figure 5.2-1. Nonreacting Swirling Combustor Flow Validation.

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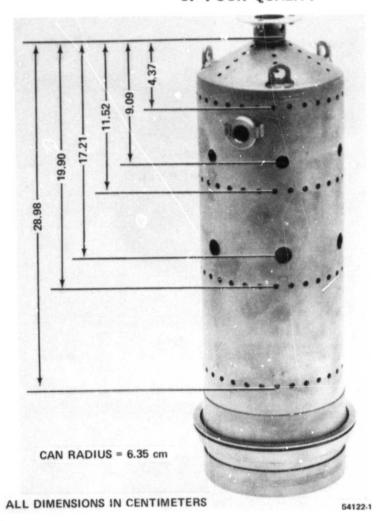


o TEST CONDITIONS

COND#	P3 (ATM)	T ₃	Waʒ (Kg/s)	<u>∆</u> P P (%)
1	10.00	288	1.818	3.25
2	10.03	288	2.263	5.01
3	9.98	288	2.736	7.39

Figure 5.2-2. Cold Flow Can Combustor Mapping Setup and Test Conditions.

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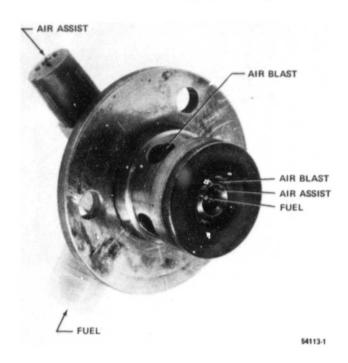


REACTING FLOW CAN COMBUSTOR GEOMETRICAL DETAILS

ORIFICE TYPE	NO. OF ORIFICES	SIZE (cm)	GEOMETRIC AREA, cm ²	AXIAL DISTANCE (cm)
DOME LOUVERS	30	0.36	3.02	_
PRIMARY	6	1.12	5.89	9.09
DILUTION	6	1.42	9.53	17.21
COOLING SLOT LIP				
#1	30	0.44	4.6	5.05
#2	30	0.48	5.43	12.20
#3	30	0.48	5.43	20.59
#4	30	0.48	5.43	29.67

Figure 5.2-3. Can Combustor for Reacting Flow Mapping.

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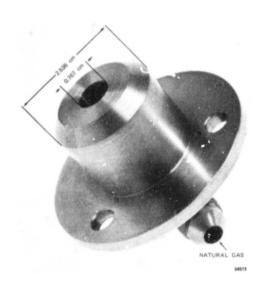


Figure 5.2-4. Natural Gas Nozzle and Airblast Nozzle Used for the Can Combustor Mapping.

A water/steam-cooled stainless steel emissions probe with ten individual radial sampling points was used for the combustion emissions mapping.

5.2.2 Annular Combustor Mapping

A reverse-flow premix/prevaporizing (PM/PV) annular combustion system that is compatible with the Garrett TFE731-2 turbofan engine envelope was designed and tested to demonstrate combustor technology capable of meeting the 1979 EPA emission standards for TI class engines as part of the NASA Pollution Reduction Technology Program. To better understand the performance characteristics of this combustion system, internal radial profiles of gaseous emissions were measured in an atmospheric test rig.

The piloted PM/PV combustion system incorporates two axially staged burning zones, as shown in Figure 5.2-5. The radial profiles of CO, CO₂, UHC, and NO_x were measured at four different axial-stations and six circumferential (θ) planes within the main combustion zone. A water/steam-cooled probe was used to obtain radial profiles. The internal emissions mapping was conducted at one atmosphere in a combustor rig without the transition liner. The effect of different parameters including combustor inlet temperature (T₃), overall fuel/air ratio, and fuel-flow splits between the pilot and PM/PV combustion zones on the emissions profiles were studied. The mapping was conducted with propane as PM/PV fuel to simulate complete evaporation; however, Jet A fuel was used for the pilot.

Information concerning the internal flow field of a TFE731 production combustor (Figure 5.2-6) was provided through measurements of ${\rm CO}_2$, ${\rm CO}$, UHC, and ${\rm NO}_{\rm X}$ taken inside the combustor primary, intermediate, and dilution zones at atmoshperic test conditions.

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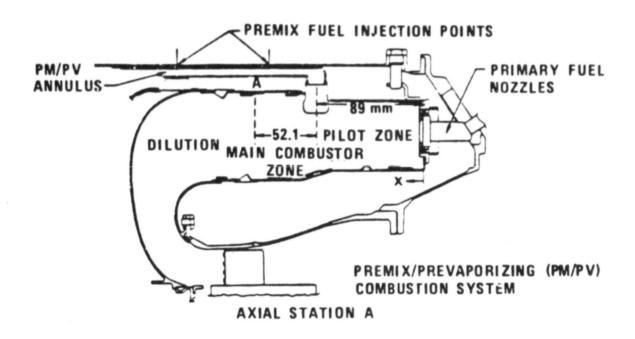


Figure 5.2-5. Axially Staged Burning Zones of the Piloted PM/PV Combustion System.

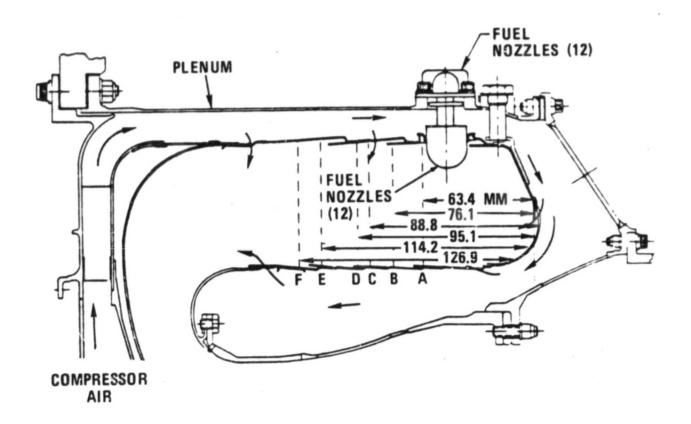


Figure 5.2-6. Emission Sampling Probe Stations Inside the TFE731 Combustor.

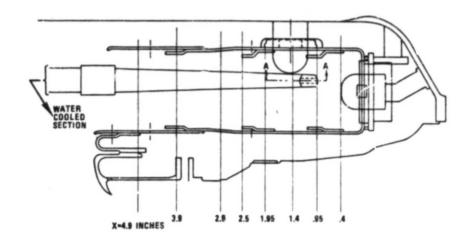
The emissions probe used for the internal mapping was the same as the one used earlier to map the PM/PV Concept 3 combustor. The eight individual sampling ports of the probe were manifolded together to obtain only averages in the radial direction. The measurements were taken at different axial stations (as shown in Figure 5.2-6) in the primary and secondary regions.

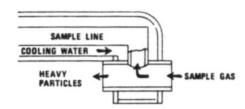
Detailed internal gaseous emissions and temperature measurements inside the Uprate T76 combustor primary zone have been conducted at various axial locations.

A single-point, water-cooled, emissions probe with an end cap (Figure 5.2-7) was designed for use in the primary zone. This probe is intended to separate relatively large liquid fuel droplets from the gas sample. The end-cap feature was also used in the construction of a ceramic radiation shield for the aspirated thermocouple used to measure primary zone temperatures.

Emissions samples were taken at five different axial positions from 1.016 to 6.35 cm from the dome. Temperature measurements were taken from the dome to the dilution zone. The measured sector extended over 36 degrees and was centered on a main fuel nozzle. Seven circumferential stations were selected to correspond with areas of carbon deposition in the Uprate T76 combustor.

Most of the data was taken at an altitude idle-engine condition and also at the sea-level design condition. Two combustors of the same part number were measured. Fuel/air ratios nearly twice the stoichiometric values were measured at the discharge of the primary zone for the design condition, indicating poor primary zone mixing.





DETAIL OF EMISSIONS PROBE END CAP - SECTION A-A

Figure 5.2-7. Schematic of Emissions Probe and Measurement Locations for Fuel/Air Rate Profiles in the UT76 Combustor.

SECTION VI

6.0 SIMPLE FLOWS

The results for the benchmark test cases (shown in Table 3) are presented in the following four categories:

- o Model evaluation for simple flows
- o Model evaluation for complex nonswirling flows
- o Model evaluation for swirling flows
- o 3-D jet-mixing flow validation

These categories are selected in increasing order of complexity and, for each category, the results will be presented for nonreacting and reeacting flows. In this section, discussion of results and model evaluation for simple flows are presented. To present the results, the predictions will be shown by lines and the data will be represented by symbols throughout this report.

6.1 Flow Over a Flat Plate

One of the benchmark test cases selected from the assembled data base is the flow over a flat plate, for which measurements were made by Watts and Brundrett⁶⁷. Their test plate was 2.44 m long with boundary layer trips placed near the leading edge to make the boundary layer fully turbulent. The mean velocity and the turbulence velocity fluctuations were measured with a hot-wire probe at x = 0.244, 0.462, 0.8466, 1.163, 1.4656 and 2.2743 m. The free stream velocity for this test case was 20.8 m/s. A schematic of this flow geometry is shown in Figure 6.1-1.

Computations for this case were made using the Garrett 2-D parabolic code, and predictions were obtained with the following models:

- o Standard k-€ model
- o Standard k-€ model with near-wall low Reynolds number correction
- o Algebraic stress model (ASM)
- o ASM with low Reynolds number correction

For all these cases, the initial conditions were applied at x = 0.244 using the measured profiles. One hundred cross-stream grid points were used in these computations. The grid distributions were selected so that the nodes were closely spaced near the wall and are farther apart near the edge of the boundary layer. For the standard $k-\epsilon$ model, the wall function treatment outlined in Section 4.2 was used to specify the wall boundary conditions.

The predicted mean velocity profiles using the standard $k-\epsilon$ model are shown in Figure 6.1-2. This figure shows that the agreement between data and predictions was poor. Problems in this computation were associated with the wall function approach for prescribing the boundary conditions at the near-wall nodes.

One way to circumvent the application of the wall functions is to apply low Reynolds number corrections to the k and ϵ equations that will enable k and ϵ to be zero at the wall in a consistent manner. From the survey of literature for low Reynolds number corrections, the model of Chien¹⁷ was selected for these computations. In Chien's model, the source terms and exchange coefficients in the k and ϵ equations have been modified. The governing equations for k and ϵ , still retain the form shown in Equation (1). The difference arises in equations (2) and (4). The modified terms in Chien's model are

$$S_{k} = G_{k} - \rho \epsilon - 2\mu \frac{k}{\gamma^{2}}$$
 (133)

and,

$$S_{\epsilon} = (C_1 G_{k} - C_2 f_{2} \rho \epsilon) \frac{\epsilon}{k} + E$$
 (134)

$$\Gamma_{\text{eff},k} = \mu + \mu_{t} f_{\mu} \tag{135}$$

where,

$$f_{\mu} = 1.0 - \exp(-0.0115 \, y^{+}),$$
 (136)

$$y^+ = \frac{\rho_U * y}{\mu}$$

$$f_2 = 1.0 - 0.2. \qquad \left[\frac{\omega_k^2}{6\mu \epsilon} \right]^2$$
 (137)

$$E = -2\mu \frac{\epsilon}{y^2} \exp \left[-0.5 \, y_+\right] \tag{138}$$

$$\Gamma_{\text{eff}, \epsilon} = (\mu_+ \mu_{\dagger})/\sigma_{\epsilon}$$
 (139)

Here, u_* is determined by using the linear part of the law of the wall,

$$v = v \cdot y_{+}, \quad 0 \le y_{+} \le 11.5$$
 (140)

With the modified terms in the k and ε equations, the wall boundary conditions at the wall (y=0) are:

$$k = 0$$

$$\epsilon = 0$$

It should be recognized that for improving near-wall solution accuracy with Chien's modification, one must employ a number of grid points inside the viscous sublayer. This is not always possible for elliptic flows. Consequently, in this report, Chien's corrections are applied only for parabolic flows. In all the computations with Chien's correction, approximately 10 nodes were distributed in the viscous sublayer.

A comparison between the data and the predicted results using Chien's correction are shown in Figure 6.1-3. A significant improvement in the agreement and predictions is obtained with the low Reynolds number correction over the wall function approach in the standard $k-\epsilon$ model.

Figure 6.1-4 illustrates the predicted results for mean velocity using the algebraic Reynolds stress model. In the ASM the value of the coefficient C_{n} is computed from equation (23) while the standard $k-\epsilon$ model assumes a constant value of $C_{D^{\bullet}}$. This parameter, C_{n} , is used for calculating the turbulence diffusion rate. Figure 6.1-4 shows that the ASM is in excellent agreement with the data of Watts and Brundrett. Application of the low Reynolds number correction on the ASM does not appreciably improve the mean velocity predictions. These results are presented in Figure 6.1-5. However, the application of Chien's low Reynolds number correction substantially improves the prediction of turbulence kinetic energy A comparison of the predicted turbulence kinetic energy profiles at x = 1.8735 m using the four models are presented in Figure 6.1-6. The predicted turbulence kinetic energy values, using the standard k- € model, are slightly higher than the measured The peak k value near the wall is significantly higher than the measurements. When Chien's low Reynolds number correction is applied to the $k-\epsilon$ model, the near-wall kinetic energy values are in better agreement with the data. The ASM predictions for k are also higher than the data, but is slightly better in comparison

with the $k-\epsilon$ model predictions. The application of the low Reynolds number correction significantly improves the predicted k values.

A comparison between data and predicted time mean fluctuating velocity components at x=1.8735 is shown in Figure 6.1-7. The ASM predicts much higher peak values for u', v', and w' components compared to the data. Application of the low Reynolds number correction yields good agreement with the data.

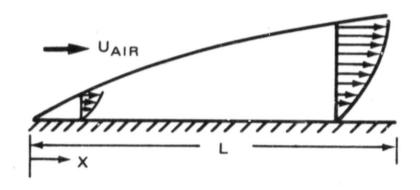
Based on the comparison between predictions and data on a flat plate turbulent boundary layer, the following conclusions can be made:

- The standard $k-\epsilon$ model gives qualitatively good results. Significant improvements in mean velocity profiles are achieved by applying Chien's low Reynolds number correction to the $k-\epsilon$ model (low Reynolds $k-\epsilon$).
- o Algebraic stress model results are as good as the low Reynolds k-€ model in regard to mean velocity profile.
- o The low Reynolds number correction is required for achieving good near-wall turbulent kinetic energy profiles with both $k-\epsilon$ and ASM models.
- o Individual fluctuating velocity components are reasonably well correlated by ASM except in the viscous sublayer, where significant improvements are obtained by applying the low Reynolds number correction.

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WATTS AND BRUNDRETT

FLOW OVER A FLAT PLATE



L = 0.23 M (U_{AIR} = 20.8 M/S L = 2.44 M

Figure 6.1-1. Waster and Brundrett 67 Setup for Turbs ant Flow over a Flat Plate.

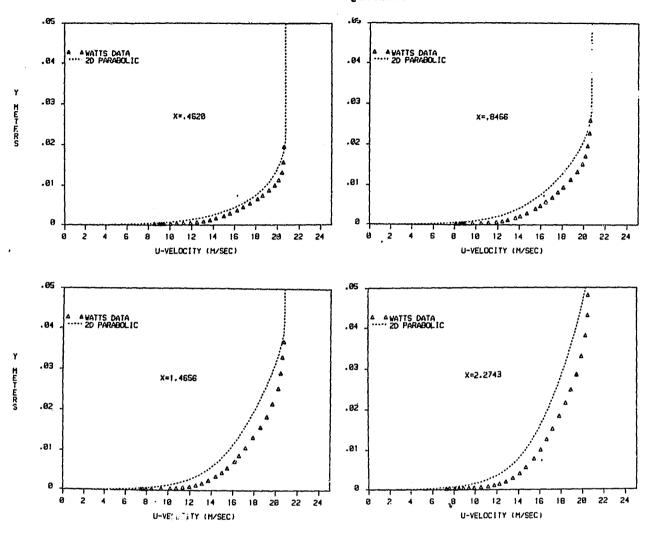


Figure 6.1-2. Turbulent Boundary Layer Mean Velocity Profiles with the Standard $k-\epsilon$ Model.

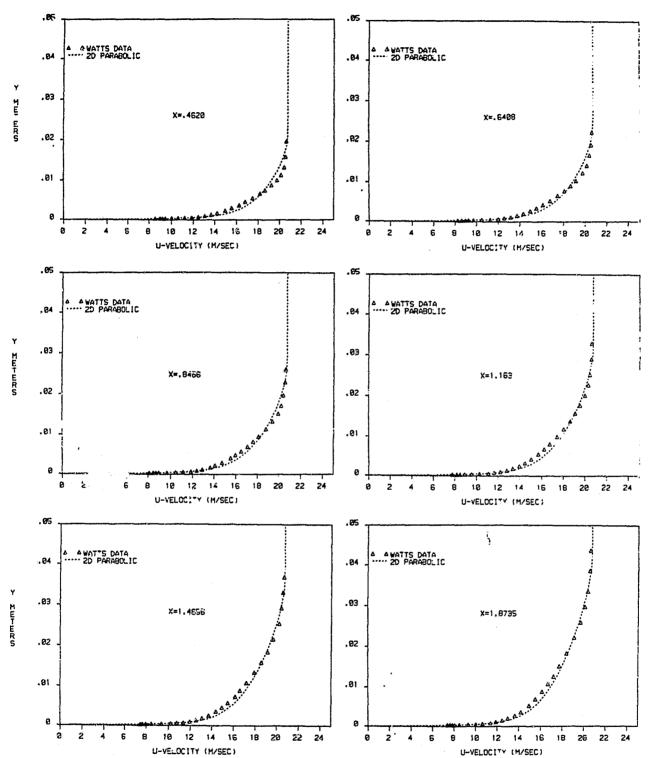


Figure 6.1-3. Turbulent Boundary Layer Mean Velocity Profiles with the $k-\epsilon$ Model and Chien's Low Reynolds Number Correction (Low Reynolds Number $k-\epsilon$ Model).

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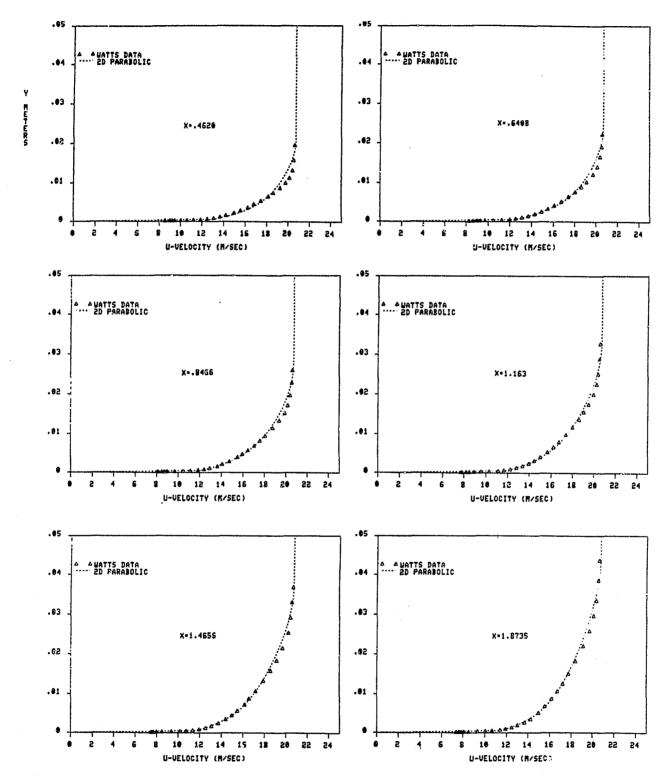


Figure 6.1-4. Turbulent Boundary Layer Mean Velocity Profiles With the Algebraic Stress Model (ASM).

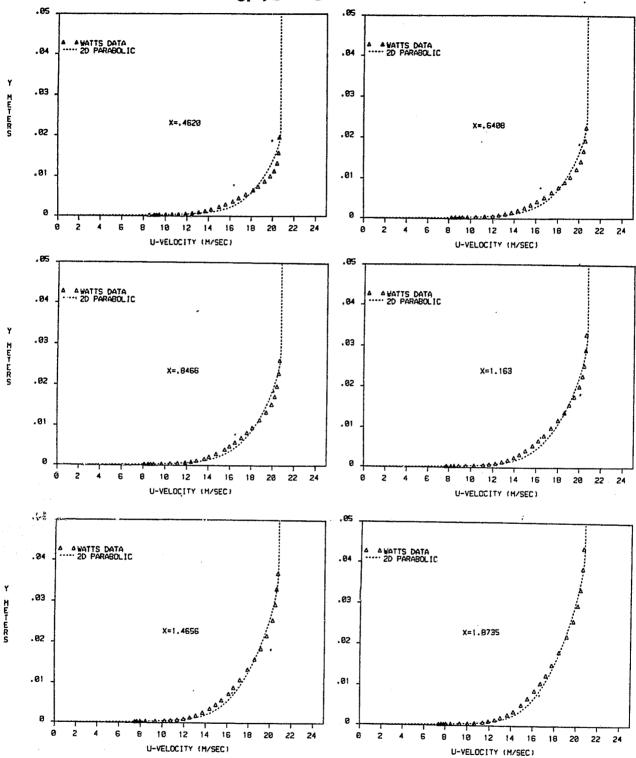


Figure 6.1-5. Turbulent Boundary Layer Mean Velocity Profiles With ASM Modified By Low Reynolds Number Correction.

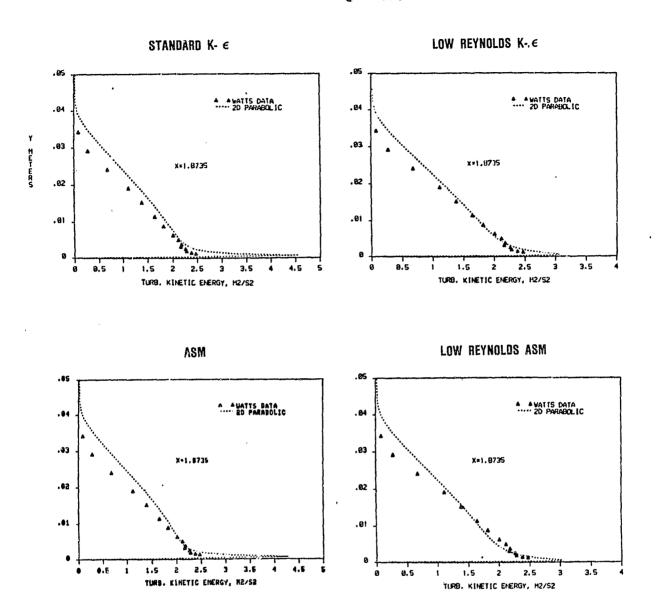


Figure 6.1-6. Turbulent Kinetic Energy Profiles Predicted By the Four Turbulence Models.

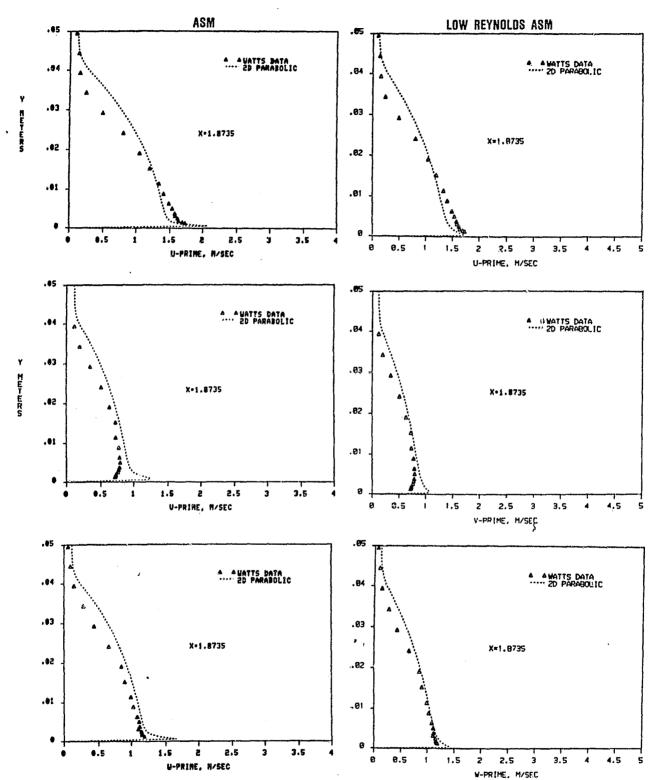


Figure 6.1-7. Fluctuating Components of Axial, Radial and Transverse Velocities (u',v' and w') Predicted by ASM, and ASM With Low Reynolds Number Correction.

6.2 Plane Couette Flow

The plane Couette flow is a well defined flow for which analytical solutions and good experimental measurements are available for evaluating the turbulence models. The test data selected for validating the models in this report were obtained by El Telbany and Reynolds²⁰⁸ in a test setup shown schematically in Figure 6.2-1. In this setup, the bottom wall was stationary and the top wall was moved at a velocity of 17.08 m/s, which corresponds to a Reynolds number of 12,640. The distance between the walls was 44 mm.

Computations for this flow were made with the standard $k-\epsilon$ model and the algebraic stress model using a 2-D parabolic code. The standard k-& model predictions and the data for mean velocity are shown in Figure 6.2-2. The agreement between data and predictions is very good. The non-dimensionalized Reynolds shear stress profile predicted by the standard k-& model is also in good agreement with the data, as seen in Figure 6.2-3. However, the profile of Reynolds stress normalized by the turbulance kinetic energy predicted by standard $k-\epsilon$ model is not in agreement with the data (Figure 6.2-4). In the standard $k-\epsilon$ model, in the regions where the shear stress is a constant, the turbulence kinetic energy is also a constant. However, the data shows a gradual reduction in the k values away from the wall with the minimum value at the plane of symmetry. Consequently, the predicted uv/k profile is contant in the core of the flow, while the data shows a gradual increase in its value away from the wall. It is possible to match the predicted and measured values of uv/k at the plane of symmetry by increasing the turbulence model constant, Cp, from 0.09 to 0.144. A significant improvement is obtained in the uv/k profile, which is shown in Figure 6.2-5. However with $C_{\rm p}=0.144$ used in the standard $k-\epsilon$ model, the predicted mean velocity profile was not in agreement with the data, as seen in Figure 6.2-6.

The ASM predictions are illustrated in Figures 6.2-7 through 6.2-13. The comparison between ASM prediction and the data for mean axial velocity is shown in Figure 6.2-7. The agreement between the two is very good. The ASM prediction for \overline{uv} , normalized by the wall shear stress is in good agreement with the data, as shown in Figure 6.2-8. However, when the Reynolds stress profiles are normalized by the local turbulence kinetic energy, shown in Figure 6.2-9, the predicted profile underestimates the values in the core of the flow. However, the ASM predictions for the centerline \overline{uv}/k values are closer to the data than that predicted by standard $k-\epsilon$ model. A very similar profile is obtained for the correlation coefficient, $\overline{uv}/(u^*v^*)$, which is shown in Figure 6.2-10. These two figures demonstrate that the ASM slightly overestimates the turbulence kinetic energy components.

The ASM prediction for the axial turbulence intensity, u', is shown in Figure 6.2-11. The predicted peak u' value is slightly smaller than the data. However, in the core of the flow, the ASM predictions are in good agreement with the data. The predicted and measured cross-stream turbulence intensity profiles are illustrated in Figure 6.2-12. The predicted v' values are about 20 percent higher than the data. The predicted w' values are also higher than the data by about 15 percent in the region near the plane of symmetry as shown in Figure 6.2-13.

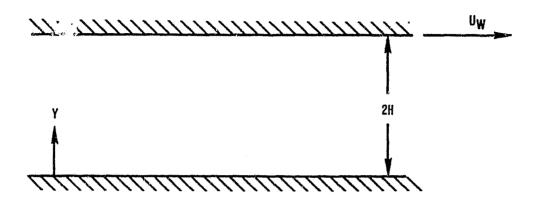
The Couette flow calculations may be summarized as follows:

- o The standard $k-\epsilon$ model predicts the mean velocity profile accurately, but underpredicts the centerline \overline{uv}/k value by about 20 percent.
- When the centerline \overline{uv}/k value is matched with the data, (using $C_D = 0.144$), the predicted mean velocity profile is in poor agreement with data.

The algebraic stress model correctly predicts the mean velocity profile and underpredicts the centerline uv/k, but the centerline uv/k values are in better agreement with the data than the standard k-ε model. The basic reason for this deficiency is because of the overestimation of v' and w' by the ASM. Overall individual turbulence components are predicted well by the ASM.

EL TELBANY AND REYNOLDS

COUETTE FLOW



2H = 0.044 M $U_W = 17.08 \text{ M/S}$
Re = $U_W H/\nu = 12,640$

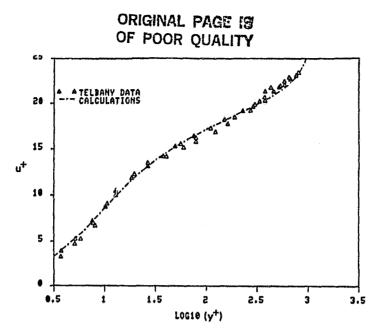


Figure 6.2-2. Comparison Between $k-\epsilon$ Predictions and Measured Couette Flow Axial Velocity Profile (u₊ versus y_+).

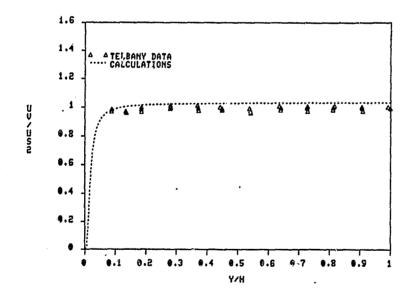


Figure 6.2-3. Comparison Between $k-\epsilon$ Model Predictions and Measured Shear Stress Profile (normalized by wall shear value).

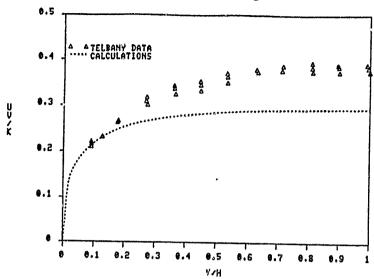


Figure 6.2-4. Shear Stress Normalized by Turbulence Kinetic Energy (uv/K) Standard $k-\epsilon$ Model With C_D = 0.09.

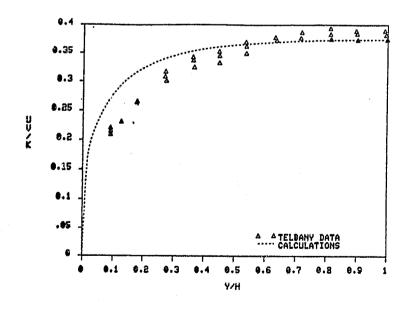


Figure 6.2-5. k- ϵ Model Predicted uv/k with $C_D = 0.144$.

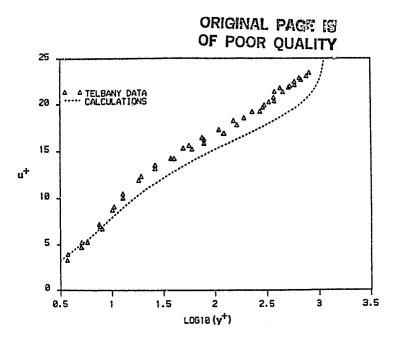


Figure 6.2-6. $k-\epsilon$ Model Predicted U₊ Profiles with C_D = 0.144.

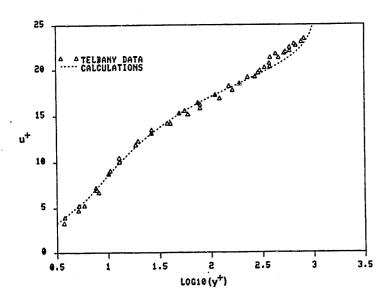


Figure 6.2-7. ASM Prediction and Measured u+ Versus y+ Profiles.

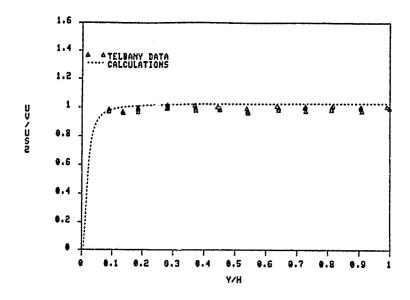


Figure 6.2-8. ASM Prediction and Measured Normalized Shear Stress Profile.

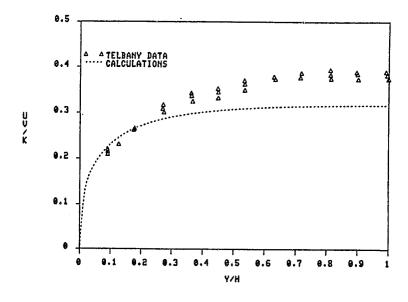


Figure 6.2-9. Shear Stress (uv) Normalized by Turbulence Kinetic Energy Predicted By ASM Versus Increased Data.

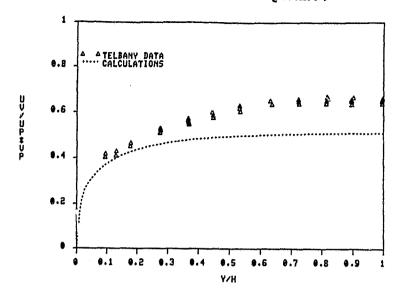


Figure 6.2-10. Correlation Coefficient (\overline{uv} /(\overline{uv} /u' x v') Predicted By ASM Versus Measurements.

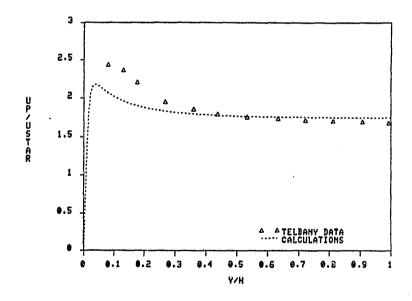


Figure 6.2-11. ASM Predictions and Measured Axial Turbulence Intensity (u'/u*).

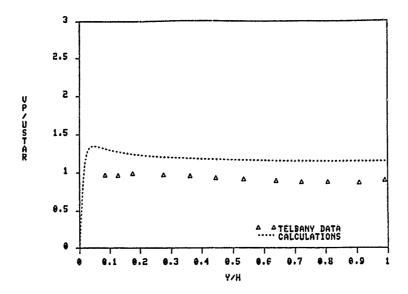


Figure 6.2-12. ASM Predictions and Measured Radial Turbulence Intensity.

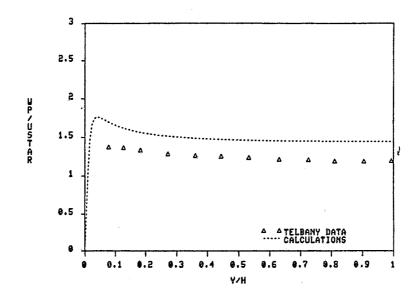


Figure 6.2-13. ASM Predictions and Measured w'.

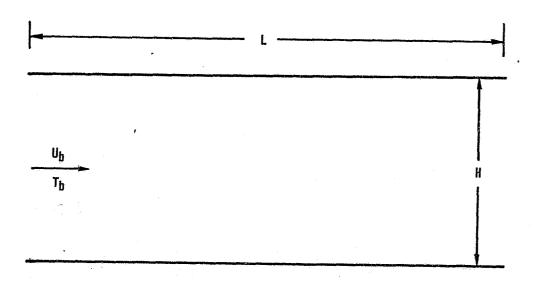
6.3 Developing Flow in a Two-Dimensional Channel

One of the simple flows considered for validating the k-€ turbulence model was the developing flow in a two-dimensional channel. Analysis of the entrance flow problem provides a means of evaluating the accuracy of the numerical scheme. Detailed mean flow measurements in the entrance region of a parallel plate were made by Emery and Gessner 65. The geometry of their test setup is shown in Figure 6.3-1. Predictions for this flow were obtained using a 2-D elliptic code with the standard $k-\epsilon$ model with 2200 grid nodes. Computations were performed until the total mass source error was less than 0.01 percent. Comparison between predicted and measured axial velocity variation along the centerline of the channel is shown in Figure 6.3-2. The difference between the two results is comparable to the measurement accuracy. Figure 6.3-3 illustrates the predicted and measured profiles of the axial velocity component at different axial stations. The agreement between data and predictions is very good.

The predicted and measured wall shear stress distributions are presented in Figure 6.3-4. The predictions and the measurements are within about 7 percent of the data, which is within the accuracy of the wall shear stress measurements. The agreement between measured and predicted results demonstrates that the standard $k-\epsilon$ model is sufficiently accurate for predicting mean flow field in a two-dimensional channel.

EMERY AND GESSNER

2-D CHANNEL FLOW



H = 0.127 M

L = 10.16 M

 $U_b = 17.85 \text{ M/S}$

 $T_b = 300 \circ K$

Re = 100,000

Figure 6.3-1. Geometry of Developing Flow in a Two-Dimensional Duet.

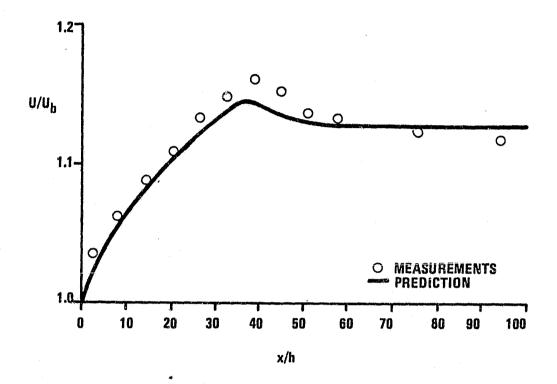


Figure 6.3-2. Predicted and Measured Distributions of Centerline Axial Velocity for Developing Flow in a Two-Dimensional Duct.

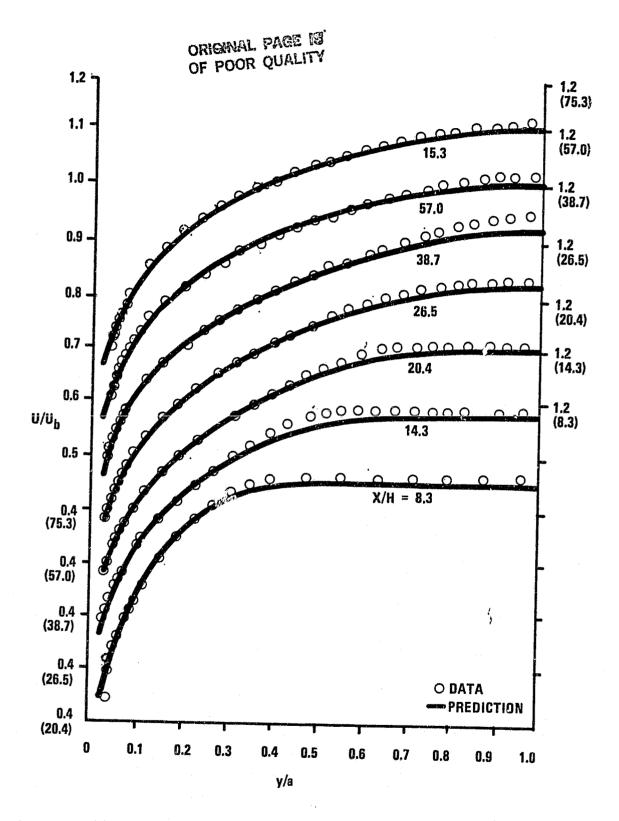


Figure 6.3-3. Predicted and Measured Mean Velocity Profiles at Different Axial Stations for Developing Channel Flow.

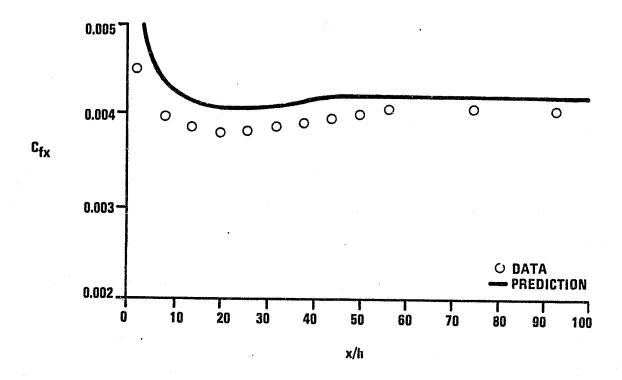


Figure 6.3-4. Predicted and Measured Wall Shear Stress Distributions for Developing Flow in a Two-Dimensional Duct.

6.4 Developing Pipe Flow

The next benchmark test case considered was the developing flow in a circular pipe. The test case selected for this problem corresponds to the measurements by Barbin and Jones⁶⁸. The geometry of their test setup is shown in Figure 6.4-1.

The bulk flow velocity at the inlet in the test case was 33.174 m/s and the Reynolds number, based upon the bulk velocity, was 388,000. The mean velocity measurements were made using pilot tubes and the turbulence velocity components were measured using an x-wire probe. Computations for this case were made using a 2-D parabolic program. The computational domain extended from x=0.3 meters to x=8.1 meters in the axial direction and from r=0 to r=0.1 meters in the radial direction. Along the axis of the tube, symmetry boundary conditions were specified, and along the pipe wall, standard wall functions were used to specify near-wall boundary conditions. In the computations, 100 grid nodal points were used in the radial direction. At x=0.3 meters, the measured profiles were used as initial profiles. Computations were made with standard $k-\epsilon$ model and ASM.

Comparison between standard $k-\epsilon$ model predictions and the data of Barbin and Jones for mean axial velocity is shown in Figure 6.4-2. The mean velocity profiles are nondimensionalized by the average bulk velocity, $U_{\rm b}=33.17$ m/s. The predicted mean velocity profiles are in very good agreement with the data.

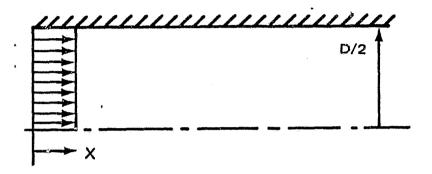
The mean axial velocity profile comparison between the data and ASM predictions is presented in Figure 6.4-3. The ASM predictions are in good agreement with the measurements. The predicted and measured root mean square (RMS) axial velocity fluctuations, u', are illustrated in Figure 6.4-4. The ASM correctly predicts the axial turbulence intensity near the axis of the pipe. Near the

wall of the pipe, predicted peak values of u' are apparently higher than the data. However, the measurements near the wall do not have sufficient resolution. The boundary conditions near the wall were specified using wall functions, which have been shown (Paragraph 6.1) to overestimate the peak turbulence kinetic energy in the case of a flat-plate boundary layer. By using an improved near-wall model, improvements in the peak turbulence intensity can be obtained. The comparison between the predicted and measured circumferential turbulence intensity component, w', is illustrated in Figure 6.4-5. These profiles have characteristics very similar to the u' profiles. The w' peak values are slightly overestimated. The near-wall model deficiencies are responsible for the overestimation of the peak w' values.

The results presented in this paragraph demonstrate that the $k-\varepsilon$ and ASM accurately predict the mean velocity profiles and that further improvements in turbulence structure and pressure drops can be achieved with an improved near-wall model.

BARBIN AND JONES

DEVELOPING PIPE FLOW



D = 0.2 M Re = 355,000 U = 33.17 M/S

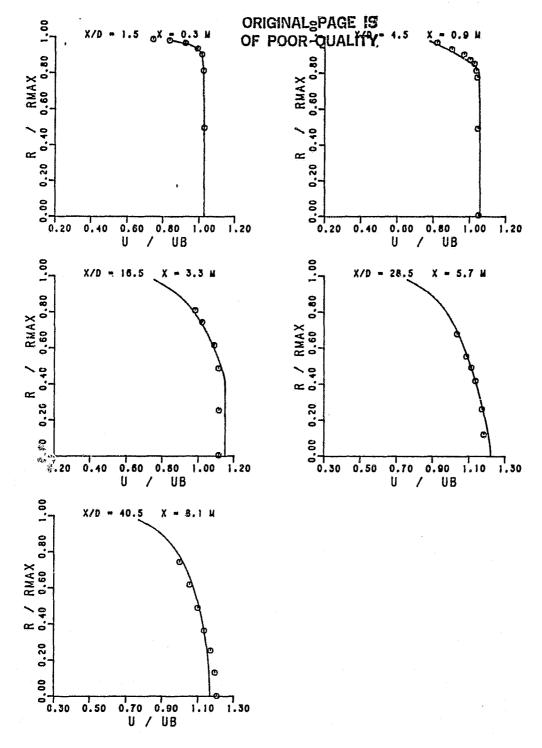


Figure 6.4-2. Comparison Between $k-\epsilon$ Model Predictions and Profiles of Axial Velocity at Different Axial Stations in a Developing Pipe Flow (U_b = The Average Flow Velocity.

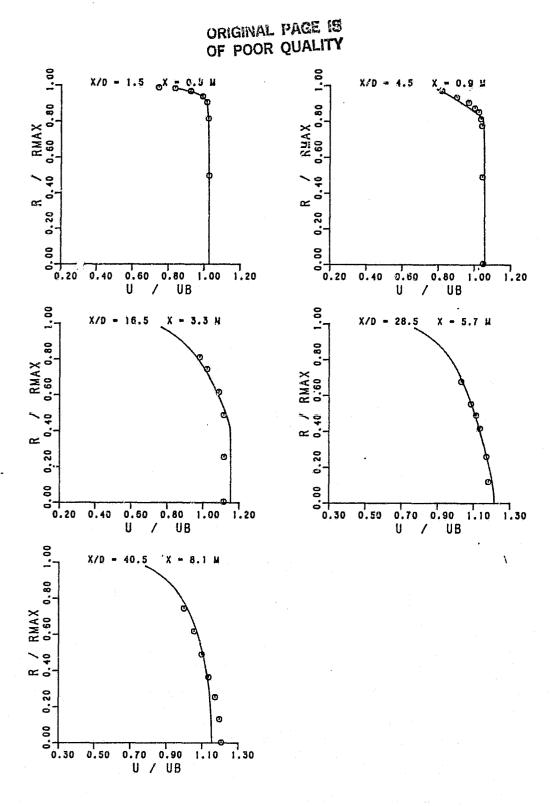


Figure 6.4-3. Comparison Between ASM Predictions and Measured Axial Velocity Profiles; D = 20 cm, $U_{\rm b}$ = 33.17 m/s.

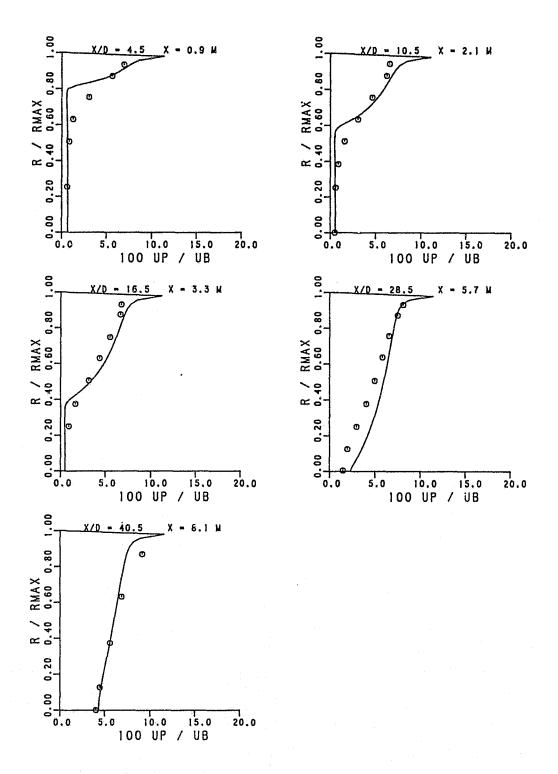


Figure 6.4-4. Comparison Between ASM Predictions and Measurements for Nondimensionalized Axial Turbulence Velocity Fluctuations.

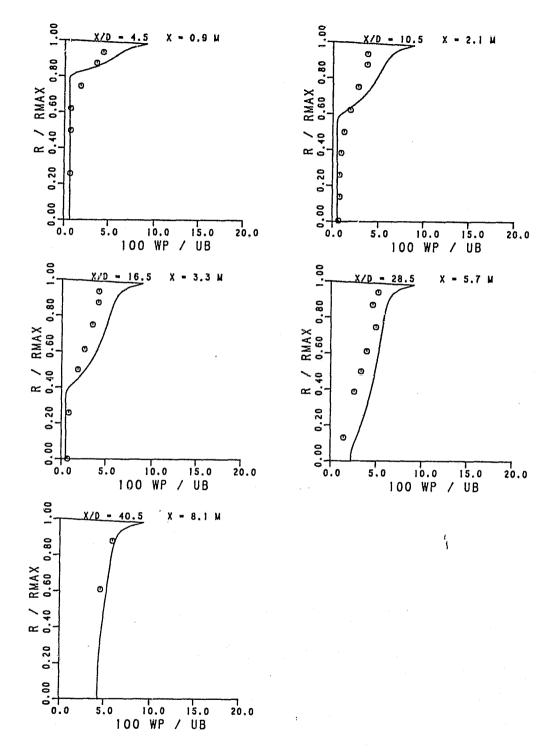


Figure 6.4-5. Comparison Between ASM Predictions and Measurements for Nondimensionalized Circumferential Turbulence Velocity Fluctuations.

6.5 Fully Developed Pipe Flow

The fully developed pipe flow is another case of simple flow where the turbulence models can be evaluated. The test measurement selected for this case was that of Laufer 209, at a Reynolds number, Ro, of 500,000. The geometry of the flow field is illustrated in Figure 6.5-1. Computations for this case were made with a 2-D parabolic program, starting with a plug flow profile at x = 0. calculations were performed up to x = 10 meters, where fully developed flow field was established. Predictions were obtained using the k-€ model and the ASM with Chien's low Reynolds number correction. A comparison between Laufer's data and the k- € model predictions are shown in Figure 6.5-2. The agreement between data and predictions is very good. The predicted and measured turbulence kinetic energy profiles are shown in Figure 6.5-3. The standard k-€ model predicts a higher value of peak turbulence kinetic energy near the wall compared to the data. Similarly, at the centerline, the $k-\epsilon$ model predicts about 40 percent higher value for k than the data.

The ASM prediction for mean velocity profile is shown in Figure 6.5-4. The predicted results and the data are in good agreement. The ASM prediction for turbulence kinetic energy is illustrated in Figure 6.5-5. The predicted peak as well as the centerline values of the turbulence kinetic energy are in good agreement with the data. The ASM predicts a faster decay of turbulence kinetic energy (k), away from the wall, but the predicted variation of k in the core of the flow is slightly smaller than the measurements.

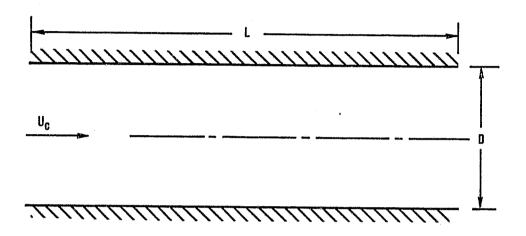
The ASM predictions for axial turbulence intensity, u', and the data are presented in nondimensional form in Figure 6.5-6. The predicted u' peak value near the wall is slightly smaller than the data. However, the agreement with data in the core of the flow is

very good. The predicted and measured v' profile is shown in Figure 6.5-7. The predicted profile is in good agreement with the data. However, the peak value of v' predicted by the model is slightly higher than the data. The predicted and measured w' profiles, shown in Figure 6.5-8, are in good agreement in the entire flow field. At the axis of the pipe, the predicted w' value is slightly higher than the data. The comparison between data and predictions for the Reynolds shear stress, uv, is shown in Figure 6.5-9. The data and predicted values are in excellent agreement.

The low Reynolds number $k-\epsilon$ model predicts the mean velocity profiles in a fully developed pipe flow accurately. It predicts a higher value of turbulence kinetic energy near the wall and at the centerline compared to the data. The ASM predicts the mean velocity profile accurately and significantly improves the turbulence kinetic energy over the $k-\epsilon$ model results.

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LAUFER PIPE FLOW



D = 0.247 M

L = 4.88 M

 $U_{\rm C} = 30.48 \ {\rm M}$

 $\cdot \text{Re} = U_0 D/v = 500,000$

Figure 6.5-1. Geometry of the Pipe Flow.

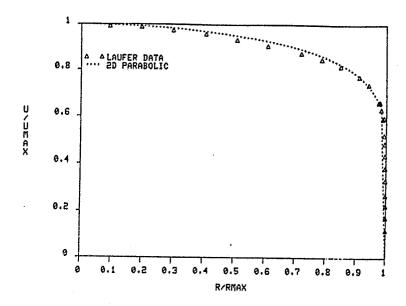


Figure 6.5-2. Low Reynolds $k-\epsilon$ Model Axial Velocity Profile.

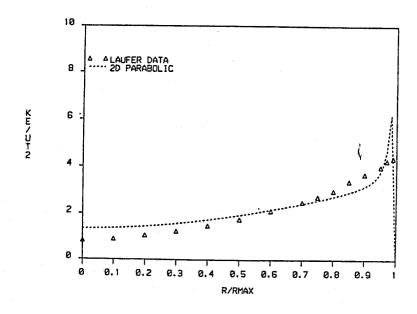


Figure 6.5-3. Low Reynolds $k-\epsilon$ Model Turbulence Kinetic Energy Profile.

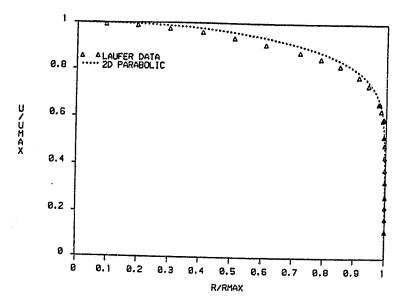


Figure 6.5-4. ASM With Low Reynolds Number Correction -- Axial Velocity Profile.

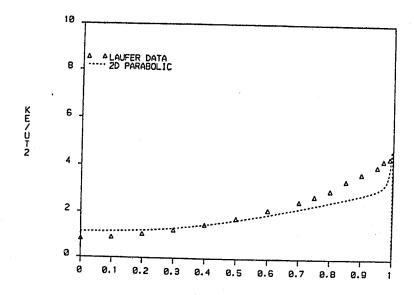


Figure 6.5-5. ASM With Low Reynolds Number Correction -- Turbulence Kinetic Energy Profile.

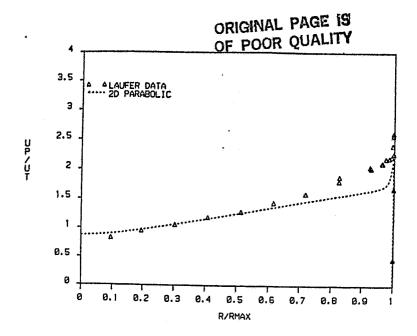


Figure 6.5-6. u'/u* Profile.

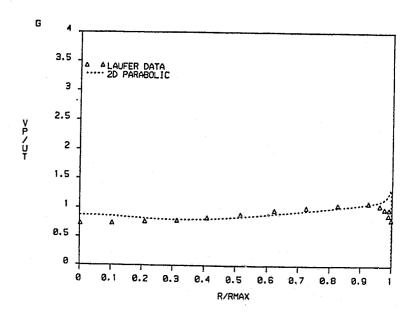


Figure 6.5-7. v'/u* Profile.

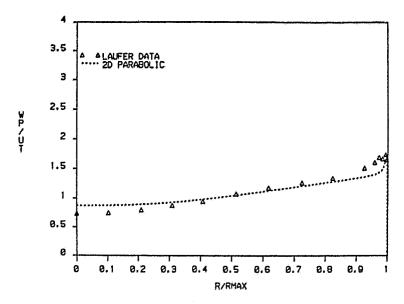


Figure 6.5-8. w'/u* Profile.

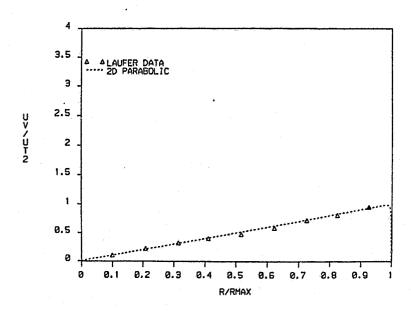


Figure 6.5-9. \overline{uv}/u_*^2 Profile.

6.6 Two-Stream Mixing Layer

Another benchmark test case selected from the data base for turbulence model validation is the flow in the mixing layer between two streams. Measurements for this case were made by Saiy and Peerless using a hot-wire probe and pitot tubes. A schematic of their flow test setup is shown in Figure 6.6-1.

Computations for this case were made using the 2-D Parabolic Program. Since this flow field does not involve a wall boundary layer, low Reynolds number correction is not needed. Predictions for this case were obtained with the standard $k-\epsilon$ model and the ASM. Initial conditions for these computations were applied at x=12.5 cm using measured data. A total of 100 cross-stream nodes were used in the computations. The nodes were closely distributed in the mixing region where gradients are higher and are sparsely spaced in the outer regions. For the test conditions, the velocities of the two streams are;

$$U_F = 16.5 \text{ m/s}; \quad U_I = 38.37 \text{ m/s}$$

The predicted mean velocity and turbulence kinetic energy profiles using the standard $k-\epsilon$ model are presented in Figure 6.6-2. The predicted mean velocity profiles are in very good agreement with the measurements. The predicted turbulence kinetic energy (TKE) values are slightly smaller than the data. However, the width of the shear layer is correctly predicted. Overall agreement between $k-\epsilon$ model predictions and data is good.

Figure 6.6-3 shows the comparison between data and predictions obtained from the algebraic Reynolds stress model for the mean velocity. The ASM predictions, similar to the $k-\epsilon$ results, are in very good agreement with data. A typical comparison between data and predicted turbulence velocity components at x=15 cm and x=15

20 cm is presented in Figure 6.6-4. The u' profiles are in very good agreement with the data. The predicted and measured v' data are in good agreement. A similar conclusion can be drawn for the w' component, with the exception that the predicted w' peak values are slightly larger than the data.

The measured data of v' and w' indicate that the peak values occur at y>o; i.e., they have shifted toward the low-velocity stream side of the mixing layer. The ASM model predicts them to lie along y=0.

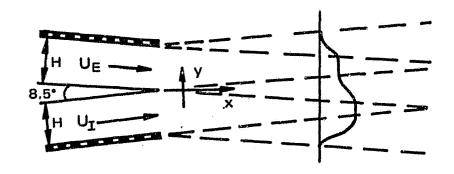
Figure 6.6-5 illustrates the comparison between data and predicted turbulence kinetic energy and shear stress (\overline{uv}) profiles at x = 15 cm and x = 20 cm. The predicted turbulence $k-\epsilon$ values are slightly smaller than the data. This is consistent with the results shown for the $k-\epsilon$ model in Figure 6.6-2. The predicted \overline{uv} profiles are in good agreement with data except for a slight discrepancy at y = 0.

Major conclusions from the mixing layer work reported here are:

- o Both k- and ASM models give equally good mean velocity profiles as well as turbulent kinetic energy profiles. The measured peak values of the turbulent kinetic energy (KE) are slightly higher than predictions; the ASM gives a little better correlation.
- o The ASM model gives good correlation for the fluctuating velocity components (u', v', and w') as well as shear stress $\overline{u'v'}$). There is slight discrepancy in regard to the radial location of the v' and w' peaks.

SAIY AND PEERLESS

TWO STREAM MIXING LAYER



H = 0.06M DUCT DEPTH = 0.30M

U_E = 10.7 M/S U_I = 25 M/S TURBULENCE INTENSITY = 0.6%

Figure 6.6-1. Two-Stream Mixing-Layer Setup of Saiy and Peerless 60.

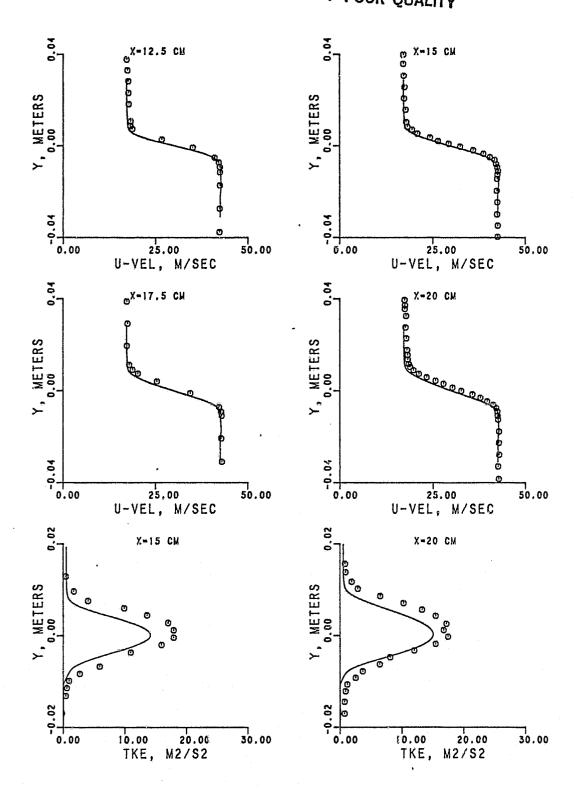


Figure 6.6-2. Mixing Layer Mean Axial Velocity and Turbulent Kinetic Energy (TKE) Profiles Predicted by the Standard $k-\epsilon$ Model.

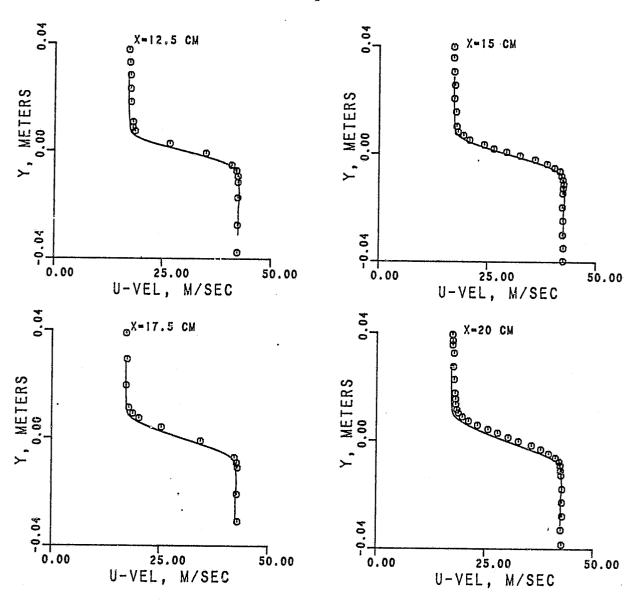


Figure 6.6-3. Mixing Layer Mean Axial Velocity Profiles Predicted by the Algebraic Stress Model (ASM).

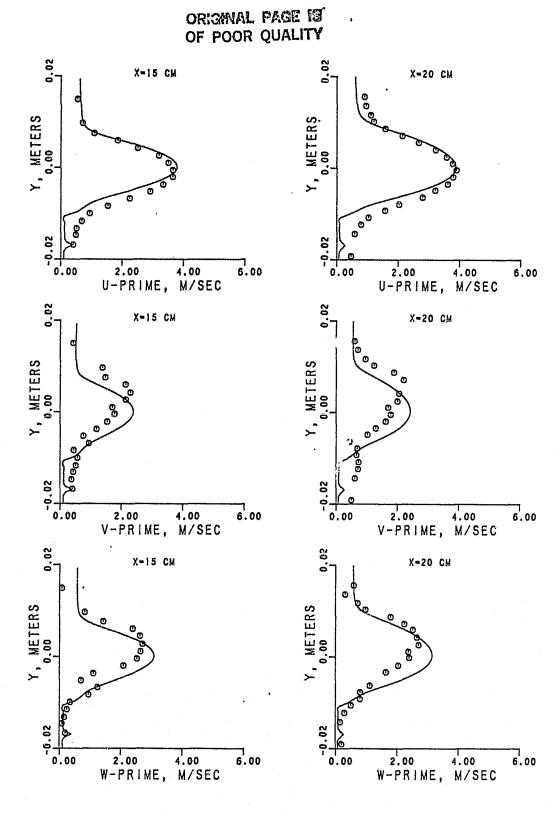


Figure 6.6-4. Mixing Layer Fluctuating Velocity Components (u', v' and w') Predicted by ASM.

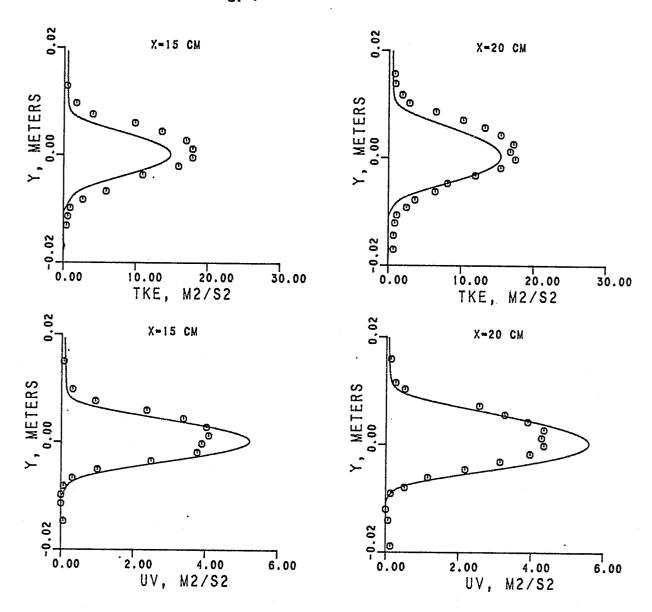


Figure 6.6-5. Mixing Layer Turbulent Kinetic Energy and Shear Stress Profiles Predicted by ASM.

6.7 Mixing of Coaxial Jets in Ambient Air

Another benchmark test case selected from the data base for turbulence model evaluations is the flow in the near field unconfined mixing region of two coaxial jets. Measurements for the selected test case were made by Champagne et al. 64 using a hot-wire probe. A schematic of their test set-up is shown in Figure 6.7-1. For the test case studied, the ratio of outer to inner velocity at the nozzle exit was 5.0 with the area ratio, $A_{\rm O}/A_{\rm i} = 2.94$.

Computations for this flow were performed using the 2-D parabolic stream with the measured inlet velocity profile at $x/D_{\rm O}$ = 1.16, where the maximum velocity, $U_{\rm max}$ was 18.29 m/s. The inlet kinetic energy profiles were obtained from measurements and a uniform inlet length scale of 0.01 $D_{\rm O}$ was prescribed. Computations were made with the standard k- ϵ model and ASM.

The predicted mean axial velocity profiles with the k- ϵ model and data are presented in Figure 6.7-2 at x/D_O = 1.16, 2.14, 3.09, 4.7, 6.05 and 8.02. The profiles shown at x/D_O = 1.16 are the initial profiles used in the computation. Here YM2 represents the local half width of the jet. These results show that the data and k- ϵ model predictions are in good agreement with each other. Figure 6.7-3 show the comparison between data and ASM predictions for mean axial velocity. These profiles are in good agreement with the data, and a slight improvement over the k- ϵ results can be seen.

Figure 6.7-4 show the comparison between the data and ASM predictions for u'. The predicted u' values are slightly higher than the data. However, the radial locations of the peak values are in good agreement with the data. Figures 6.7-5 presents the comparison of the v' profiles. The predicted results and measurements are again in good agreement. The comparison between predicted \overline{uv} and measured values are illustrated in Figure 6.7-6. These two results

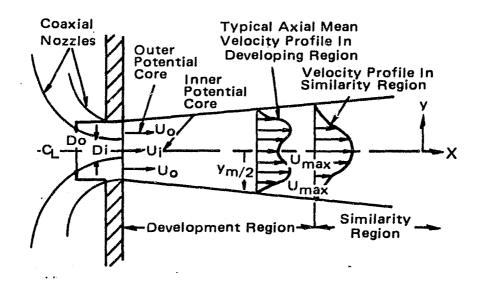
are in very good agreement with each other up to x/D = 4.07. Beyond this station, the predicted \overline{uv} values are slightly larger in magnitude compared to the data.

The $k-\epsilon$ and ASM predictions are in good agreement with measurements. Further improvements in ASM predictions can be achieved by fine tuning the empirical constants in the model.

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CHAMPAGNE AND WYGNANSKI

MIXING OF TWO COAXIAL JETS IN AMBIENT AIR



 $D_1 = 0.0254M$

 $D_0 = 0.0435M$

 $U_0 = 37.4 \text{ M/S}$

 $U_I = 7.5 \text{ M/S}$

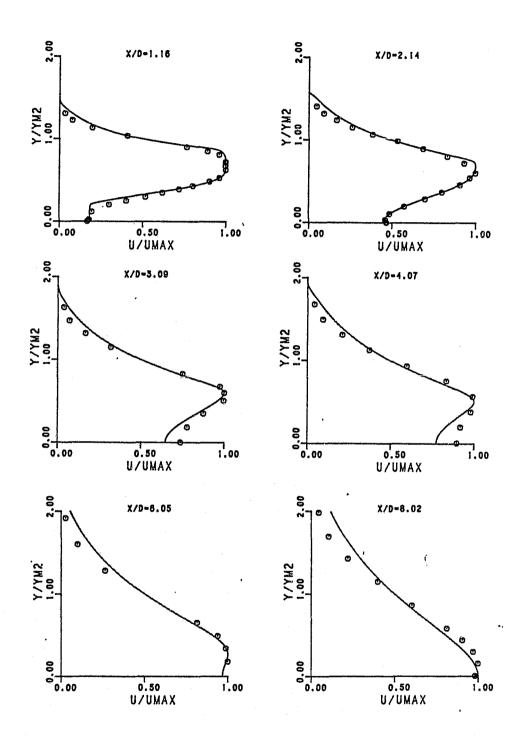


Figure 6.7-2. Comparison Between $k-\varepsilon$ Model Predictions and Measured Axial Velocity Profiles of Coaxial Jets in Ambient Air.

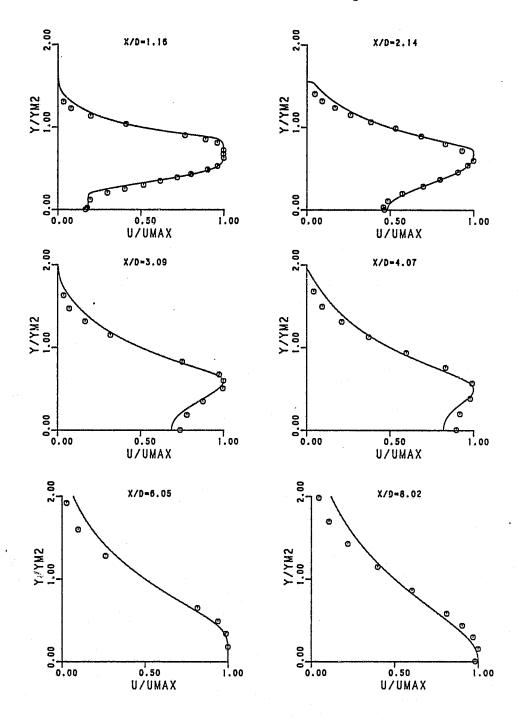


Figure 6.7-3. Comparison Between ASM Predictions and Measured Axial Velocity Profiles of Coaxial Jets in Ambient Air.

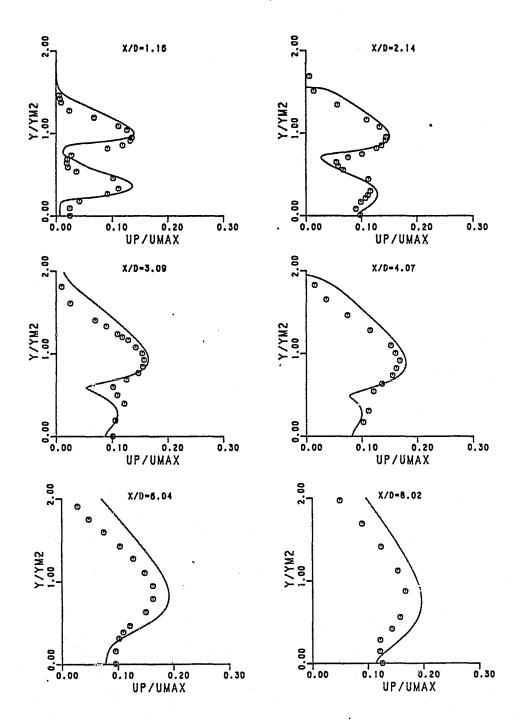


Figure 6.7-4. Predicted and Measured Profiles of RMS Axial Velocity (u') for Coaxial Jets in Ambient Air.

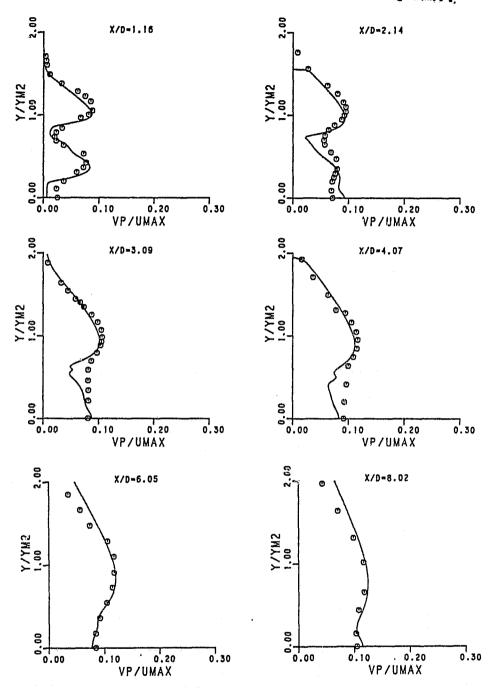


Figure 6.7-5. Predicted and Measured Profiles of Fluctuating Radial Velocity Component (v').

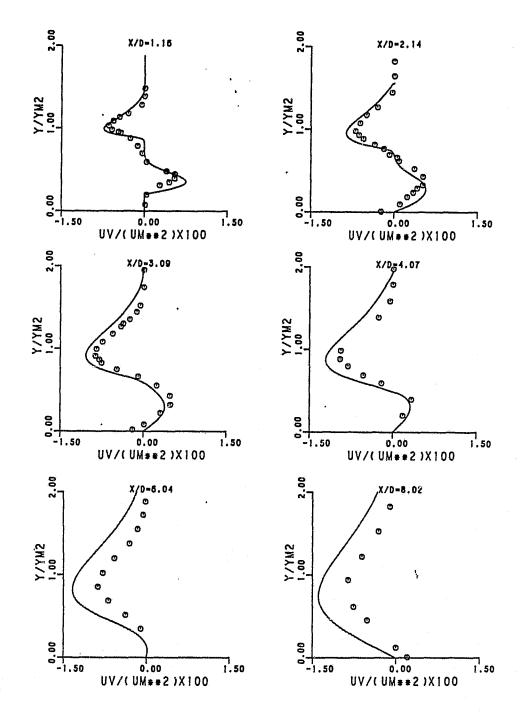


Figure 6.7-6. Predicted and Measured Sheer Stress (uv) Profiles for the Coaxial Jets in Ambient Air.

6.8 Free Circular Jet

In partial support of the free swirling jet correlation and to further elucidate the coaxial jet mixing, a simpler case of free circular jet was selected for model validation. The benchmark case selected for this flow was that of Wygnanski and Fiedler 210 . They have reported accurate measurements of mean and turbulence velocity components using a hot-wire anemometer in a test setup shown schematically in Figure 6.8-1. Their jet diameter at the nozzle exit was 26.4 mm with a jet exit velocity of 51 m/s. Measurements were made at x/D = 40, 50, 60, 75, and 97.5. Computations for this case were made with a 2-D parabolic program using initial profile obtained from measurements at X/D = 40. Along the axis of the tube, symmetry conditions were applied. A total of 100 cross-stream points were used in the computations.

The mean axial velocity profiles obtained from measurements and standard k- ϵ model predictions are shown in Figure 6.8-2. The top left corner figure shows the initial profiles used in the computations. The predicted axial velocity results show a slower decay of centerline velocity than the measurements do. This may be due to under-estimated diffusion rates. Launder 211 has recommended modifying the turbulence model constants C_D and C_2 for round jets in stagnant surroundings according to the relation

$$C_D = 0.09 - 0.04 f$$
 (141)

$$C_2 = 1.92 - 0.067 f$$
 (142)

$$f = \frac{\Delta y}{2U} \left| \frac{\partial U_{\mathbb{C}}}{\partial x} - \left| \frac{\partial U_{\mathbb{C}}}{\partial x} \right| \right|^{0.2}$$
 (143)

These modifications were used to predict the structure of Wygnanski and Fiedler's free jet. Comparison between the data and predictions for mean axial velocity are shown in Figure 6.8-3. The

predicted centerline velocity decay rate shown in this figure is smaller than the standard $k-\epsilon$ model results.

The correction factor f is always positive and equations (141) and (142) would tend to reduce the magnitudes of \mathbf{C}_{D} and \mathbf{C}_{2} . Reduction of \mathbf{C}_{D} value would tend to reduce the eddy viscosity with attendent decrease in mixing rate.

The present approach is to increase the $\mathbf{C}_{\mathbf{D}}$ value by the expression

$$C_D = 0.09 + 0.04 f$$
 (144)

Furthermore, it was considered necessary to evaluate separating the effects of changing C_C and C_2 . Application of equation (144) alone on the $k-\epsilon$ model will be denoted as the $k-\epsilon$ 1 model and the use of equation (144) and (142) will be denoted as the $k-\epsilon$ 2 model in this report.

The predicted axial velocity profiles using the $k-\epsilon 1$ model and the measurements are presented in Figure 6.8-4. The agreement between data and the $k-\epsilon 1$ model is excellent. Figure 6.8-5 allows the $k-\epsilon 2$ model predictions for axial velocity. These results demonstrate that the $k-\epsilon 2$ model tends to overestimate the mixing, which is responsible for the fast decay of the centerline velocity of the jet.

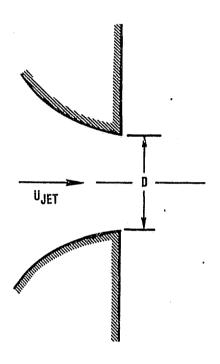
The predicted mean velocity using the standard ASM is presented in Figure 6.8-6. The ASM tends to slightly underestimate the mixing of the jet compared to the $k-\epsilon l$ model, but is significantly better than the standard $k-\epsilon$ model. Comparison of the predicted u' profiles and measurements, as shown in Figure 6.8-7, illustrates that u' is underpredicted up to x/D=60 and beyond that station the agreement between data and ASM predictions is very good. This is a consequence of the underestimated mixing

rates in the model. Figure 6.8-8 shows the comparison of the predicted and measured v' component at three axial stations. The agreement between these two is quite good. However, some disagreements can be seen close to the axis of the jet. The predicted w' velocity profiles are in good agreement with the data, as seen in Figure 6.8-9. The predicted \overline{uv} profiles are compared with the measurements in Figure 6.8-10. The \overline{uv} values are initially underpredicted and are slightly overestimated at x/d = 75.

For the case of the round free jet, the standard $k-\epsilon$ model tends to underestimate the turbulent diffusion rates. Modifications of the empirical constants are necessary to improve these results. The $k-\epsilon l$ model accurately predicts the mean velocity profiles, while the $k-\epsilon 2$ model tends to overestimate the jet centerline decay rate. The ASM shows a substantial improvement over the standard $k-\epsilon$ model and no ad hoc modification of the empirical constants is necessary. The turbulence structure is well predicted by the ASM, and further refinement of the ASM is necessary to improve the quantitative predictions.

WYGNANSKI AND FIEDLER

AXISYMMETRIC FREE JET



D = 0.0264 M U_{JET} = 51 M/S T_{JET} = 300° K

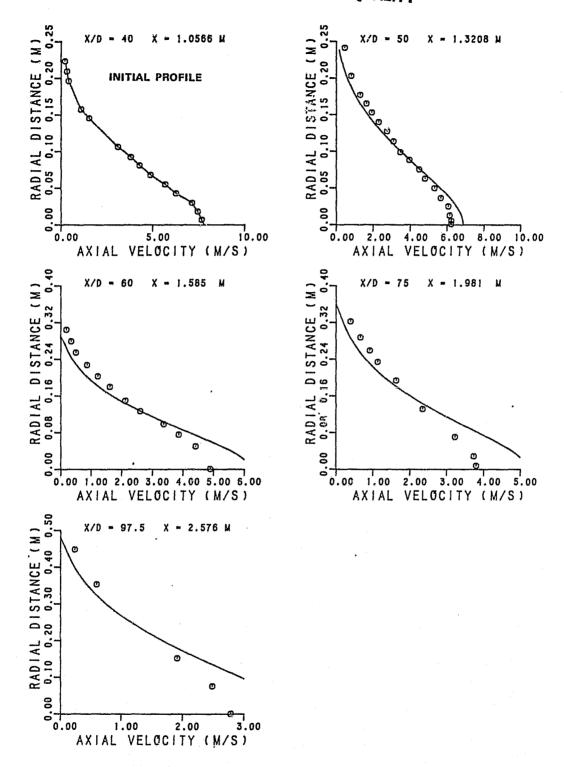


Figure 6.8-2. Comparison Between $k-\epsilon$ Model Predictions and Measured Axial Velocity Profiles, Initial Jet Velocity = 51 m/s Initial Jet Diameter D = 26.4 mm.

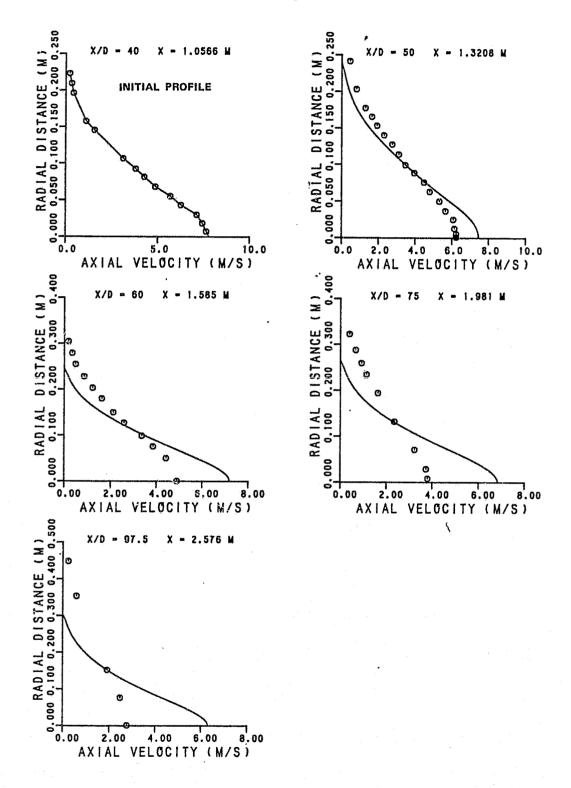


Figure 6.8-3. Modified $k-\epsilon$ Model Predictions with C_D and C_2 Constants Given by Equations (141) and (142).

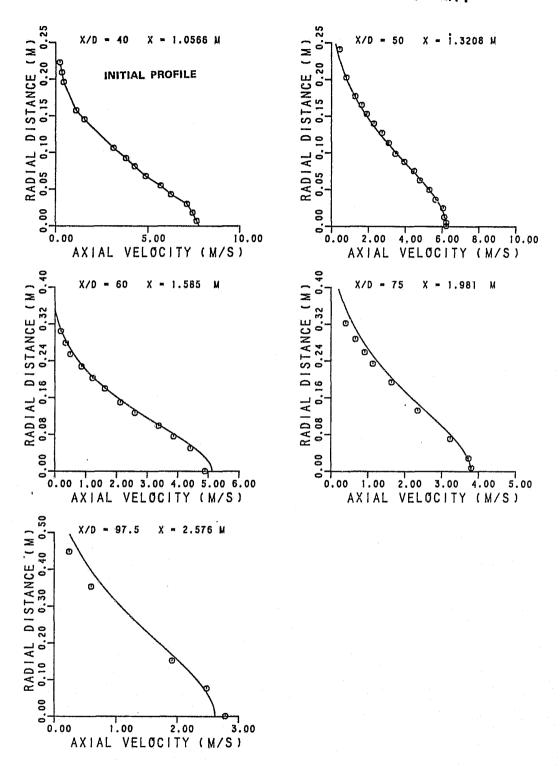


Figure 6.8-4. Modified $k-\epsilon$ Model $(k-\epsilon 1)$ Predictions With C_D as given by Equation 62.

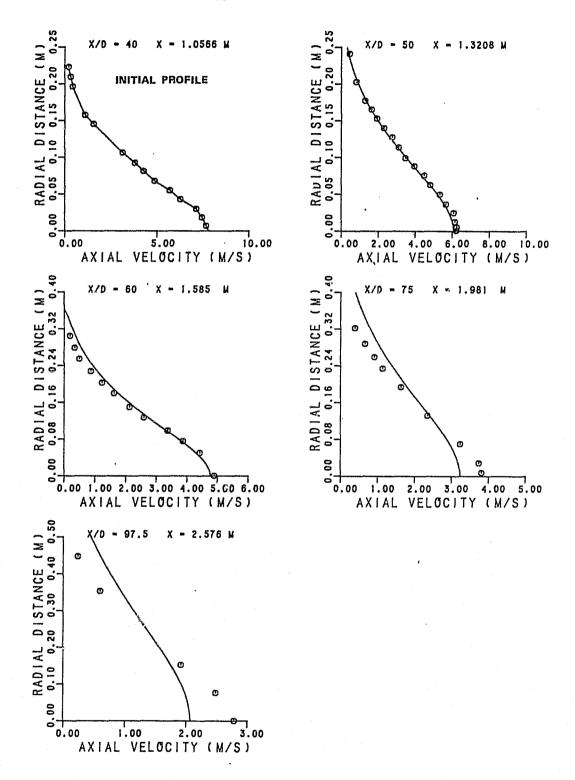


Figure 6.8-5. Modified $k-\epsilon$ Model $(k-\epsilon 2)$ Predictions with C_2 and C_D As Given by Equations 60 and 62.

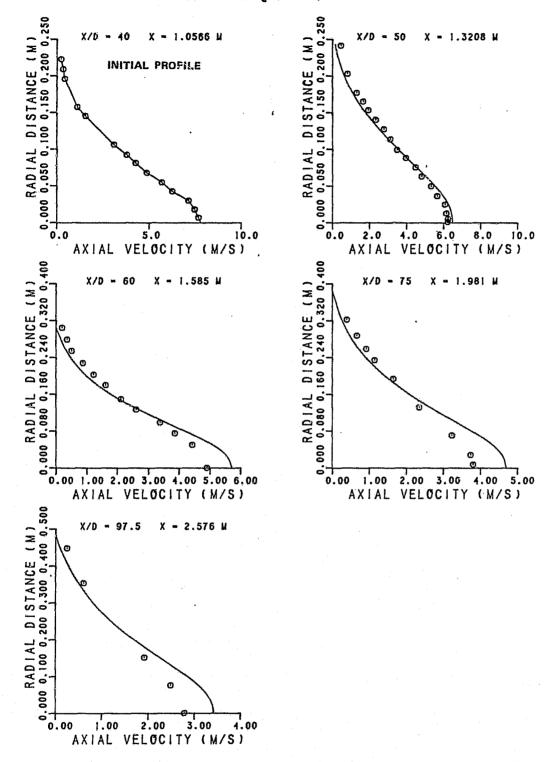


Figure 6.8-6. Comparison Between ASM Predictions and Measured Axial Velocity Profiles of a Free Jet.

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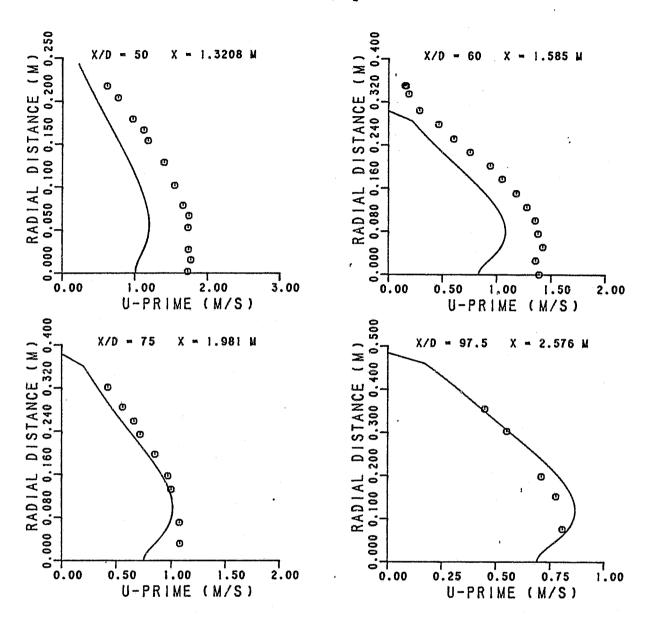
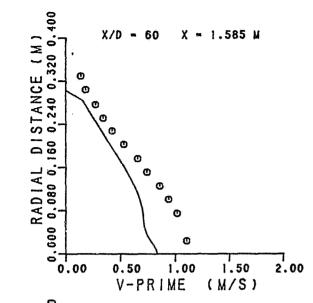
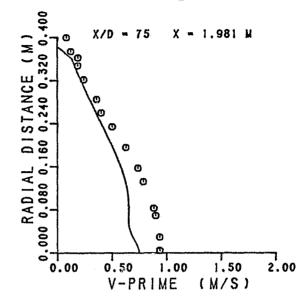


Figure 6.8-7. Comparison Between ASM Predictions and Measurements for Axial RMS Turbulence Velocity Fluctuations.





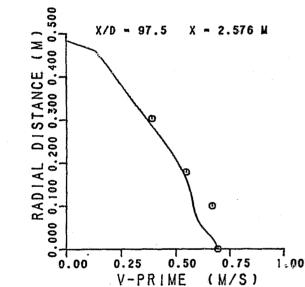


Figure 6.8-8. Comparison Between ASM Predictions and Measurements for Radial RMS Turbulence Velocity Fluctuations.

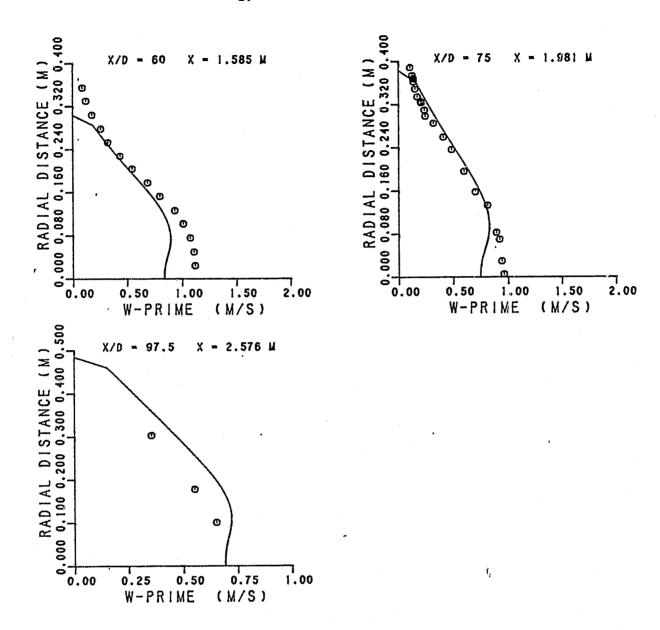


Figure 6.8-9. Comparison Between ASM Predictions and Measurements for Circumferential RMS Turbulence Velocity Fluctuations.

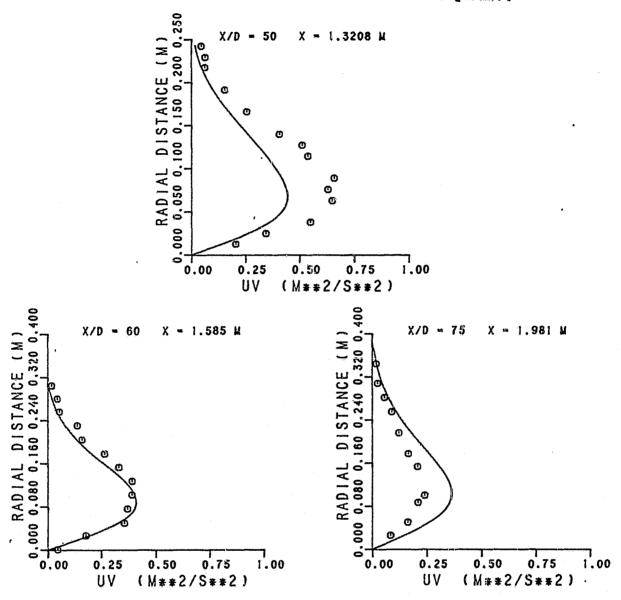


Figure 6.8-10. Comparison Between ASM Predictions and Measurements for Turbulent Shear Stress.

6.9 Flow Over a Heated Flat Plate

The $k-\epsilon$ and the ASM seem to predict the momentum transport reasonably well for simple flows. It was deemed essential to evaluate these models on the transport of scalar quantities such as temperature. The benchmark test case that was selected for this purpose was the flow over a heated flat plate. Measurements of mean and fluctuations of temperature were made for this case by Charnay 110 et al. A schematic of their setup is shown in Figure 6.9-1. The flat plate was heated from the leading edge up to x=0.7 m and maintained at a uniform temperature of 313°K. Beyond x=0.7 m, the wall temperature was abruptly changed and maintained at 290°K. The free stream temperature of air during the test was 293°K. Measurements of \overline{T} , $\overline{T}^{1/2}$ and $\overline{v}\overline{T}^{1}$ were made at x=0.7, 0.8, 0.9, 1.05, and 1.4 m.

Computations for this case were made using the 2-D parabolic program with the initial conditions specified at x=0.7 m from the measured profiles. At x=0.7 m, only the measured temperature profiles were reported. The inlet velocity profiles were assumed to conform to the law of the wall. The unknown wall mean stress was calculated by assuming the temperature distribution to also follow a logarithmic law. The details of this calculation procedure are as follows:

For a flat plate with constant free stream velocity and surface temperature, the local Stanton number $(\frac{h}{\rho_\infty U_\infty C_p})$ is given by Kays 212 as

St =
$$\frac{0.0287 \text{ Re}_{x}^{-0.2}}{0.169 \text{ Re}_{x}^{-0.1} (13.2 \text{ Pr}-10.16) + 0.9}$$
(145)

where
$$R_{e_x} = \rho_{\infty} U_{\infty} x/\mu$$

For the given free stream conditions, St was computed. The local wall heat flux, $\mathbf{q}_{\rm w}$ was obtained from 212

$$q_W = \rho_\infty C_D U \quad (T_W - T_\infty) \quad St$$
 (146)

The logarithmic law for temperature is given by Kays 212 as

$$t_{+} = 2.195 \ln y^{+} + 13.2 Pr - 5.66$$
 (147)

where,

$$t^{+} = \frac{(T_{w}^{-T}) u_{*}}{(q_{w}^{\prime}/\rho_{\infty}C_{p})}$$
 (148)

and

$$y = \frac{\rho_{\infty} u_{*} y}{\mu} \tag{149}$$

From the prescribed temperature profile (T vs. y), using equation (148), the value of u_* was computed. Knowing u_* , the velocity profile was constructed from the law of the wall for mean velocity. This profile was used as the initial velocity profile. The turbulence kinetic energy was assumed to be a constant with $k=0.003~\mathrm{U}^2$. The length scale was assumed to be linear, $1=\kappa y$ up to $y=\delta$. Beyond that point, 1 was set equal to $\kappa\delta$.

The boundary condition on the boundary layer edge was specified through the computed entrainment rate. Along the wall boundaries, Chien's low Reynolds number correction to the $k-\epsilon$ model was applied. Across the boundary layer, a total of 100 nodes were distributed with the nodes closely spaced near the wall and further apart near the boundary layer edge. Computations were made using

- o k-€ model with gradient transport model
- o ASM with gradient transport model

o Algebraic scalar transport model (ASTM)

The standard $k-\epsilon$ model predictions with gradient scalar transport model are presented in Figures 6.9-2 through 6.9-4. In gradient transport assumption, the following expressions were used for the turbulent transports:

$$\rho \overline{u\theta^{\dagger}} = - \Gamma_{\text{eff},\rho} \frac{\partial \theta}{\partial x}$$
 (150)

$$\rho \overline{v\theta'} = -\Gamma_{\text{eff}} \frac{\partial \theta}{\partial r} \tag{151}$$

$$\frac{\overline{\theta'^{2}}}{\theta'^{2}} = \frac{2}{a_{\theta}} \frac{k}{\epsilon} \Gamma_{\text{eff}} \left\{ \left(\frac{\partial \overline{\theta}}{\partial x} \right)^{2} + \left(\frac{\partial \theta}{\partial r} \right)^{2} \right\}$$

$$\Gamma_{\text{eff}} = \frac{\mu_{\text{eff}}}{Pr_{\text{eff}}}$$
(152)

where

$$Pr_{eff} = 0.9$$

Figure 6.9-2 shows the comparison between measured and predicted mean temperature profiles across the boundary layer. In these figures, the abscissa represents the temperature difference, $(T-T_{W_O})/(T_{\infty}-T_{W_O})$, where T_{W_O} is the wall temperature upstream of X=0.7 m (313°K). At X=0.7, the nondimensional temperature profile would be similar to the velocity profile with a monotonic variation between zero at the wall to 1.0 at face stream edge. Just downstream of X=0.7, the value of the nondimensional temperature at the wall jumps to 1.15. The mean temperature profiles gradually recover from a hot wall condition to a cold wall profile. The $k-\epsilon$ model predictions for temperature differences are smaller than the data as seen in Figure 6.9-2. In other words, the model underestimates the heat transfer rate to the wall.

The root mean square (RMS) value of the temperature fluctuations obtained from the $k-\epsilon$ model are shown in Figure 6.9-3. In

these figures, the T' values are nondimensionalized by $(T_{W_O}-T_{\infty})$, $(20^{\circ}\text{K}\text{ in the present case})$. The k- ϵ model predicts high values of T' near the wall. At the outer edge of the boundary layer, the k- ϵ model predictions are in reasonably good agreement with data. At x = 140 cm, the peak T' values tend to approach the measured values. This indicates that the gradient diffusion assumption is valid for equilibrium boundary layers.

Figure 6.9-4 illustrates the comparison between data and k- ϵ model predictions for the turbulent transport \overline{vT} . In these figures, the quantity \overline{vT} is nondimensionalized by U $(T_{W_O}-T_{\infty})$, with T_{W_O} being the wall temperature upstream of x = 0.7 m. The k- ϵ model underestimates the heat flux component \overline{v} , especially in the region close to the wall.

The predicted mean temperature profiles obtained from the ASM and gradient transport assumption are shown in Figure 6.9-5. These profiles are almost identical to those obtained from the $k-\epsilon$ model, and the temperature differences are overestimated. The ASM predictions for RMS temperature fluctuations are shown in Figure 6.9-6. These profiles are also identical to those obtained from $k-\epsilon$ model. A similar conclusion may be drawn for the \overline{vT} profiles obtained from ASM, as seen in Figure 6.9-7. These figures illustrate that the gradient transport model underestimated the heat flux, and the ASM does not significanlty improve the heat estimation.

The predicted results using the ASTM are presented in Figure 6.9-8 through 6.9-10. The ASTM uses the expressions given in Section 4.0 for the various turbulent transports. The ASTM predictions for mean temperature are shown in Figure 6.9-8. Comparison with the $k-\epsilon$ model results (Figure 6.9-2) shows that the ASTM significantly improves the predictions for mean temperature, and at x = 140 cm, the predicted mean temperature profile agrees very well with the data.

The ASTM predictions for RMS temperature fluctuations are illustrated in Figure 6.9-9. The ASTM tends to overestimate the T' values near the boundary layer edge. In the near-wall region, some differences between the data and ASTM predictions are present. These differences are mainly due to the estimated turbulence structure, namely, u^2 and v^2 profiles.

The ASTM predictions for the heat transport \overline{vT} are presented in Figure 6.9-10. These profiles are in good agreement with the data near the edge of the boundary layer. However, some differences exist in the near-wall region. These are due to the differences between estimated values and test conditions. The test results for the turbulence velocities were not reported. Further improvements in the ASTM predictions can be achieved if the turbulence structure predictions are refined.

The results presented in this paragraph show that even for a simple flow case of boundary layer with sudden changes in wall temperature, the gradient transport assumption is not valid. The ASTM gives significantly improved predictions. Further improvements in the Reynolds stress predictions are needed to obtain quantitatively accurate results from ASTM.

Comparisons of mean temperature $(T-T_{W_O})$, the RMS temperature fluctuations (T^*) , and the heat transport $(\overline{v/T^*})$ calculated using the various models can be made from the following figures:

	<u>Figures</u>
$\mathbf{T}\mathbf{-T_{W_{O}}}$	6.9-2
0	6.9-5
	6.9-8
Tr t	
$rac{ extbf{T'}}{ extbf{Tw}_{ extsf{O}}- extbf{T}_{\infty}}$	6.9-3
- "O -∞	6.9-6
	6.9-9
VT T	
$U_{\infty} (T_{W_{\mathcal{O}}} - T_{\infty})$	6.9-4
-50'-MO -00'	6.9-7
	6.9-10

CHARNAY ET AL

FLOW OVER A HEATED FLAT PLATE

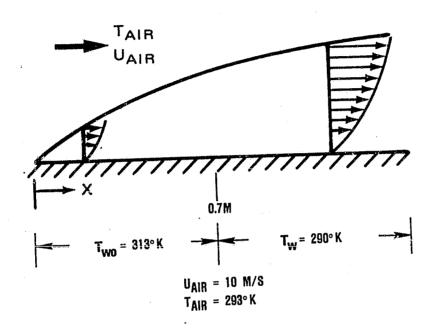


Figure 6.9-1. Geometry of Flow Over a Flat Plate with Step Change in Temperature.

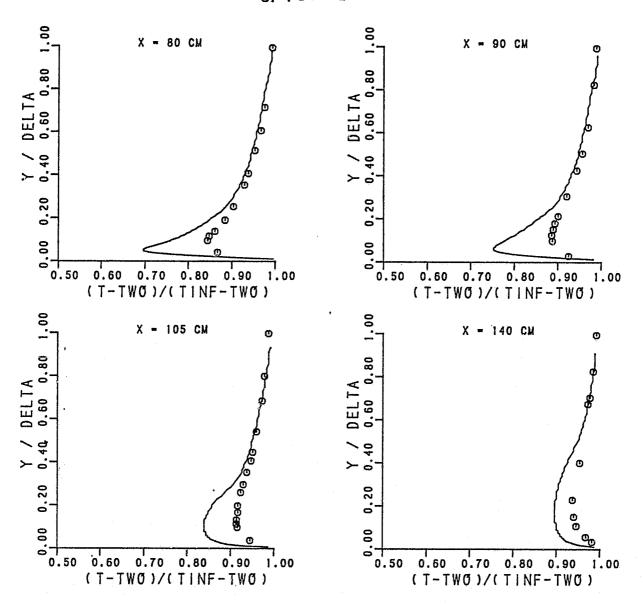


Figure 6.9-2. $k-\epsilon$ Model Predictions and Measured Mean Temperature Profile on a Flat Plate with Step Change in Temperature.

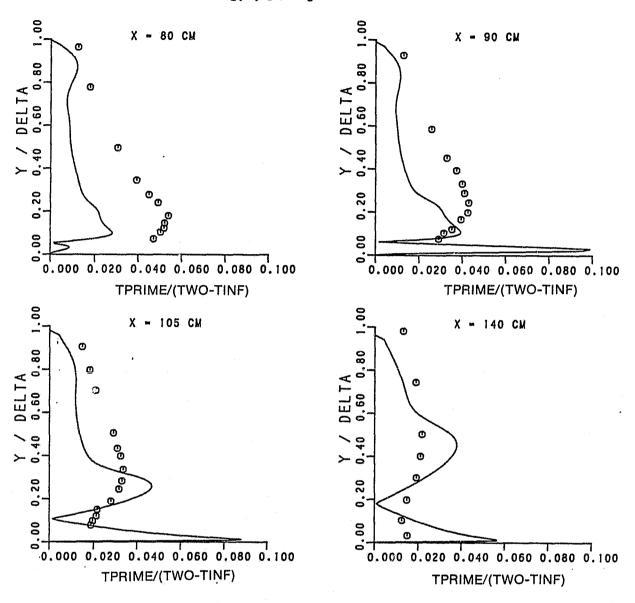


Figure 6.9-3. k- ϵ Model Prediction, and Measured RMS Temperature Normalized by (T $_{WO}$ - T $_{\infty}$).

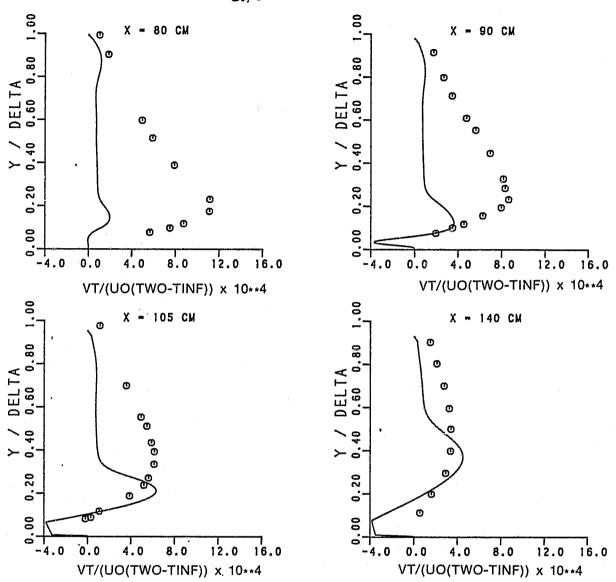


Figure 6.9-4. k- ϵ Model Predictions and Measured (vT') Normalized by U $_{\infty}$ (T $_{\rm WO}$ - T $_{\infty}$).

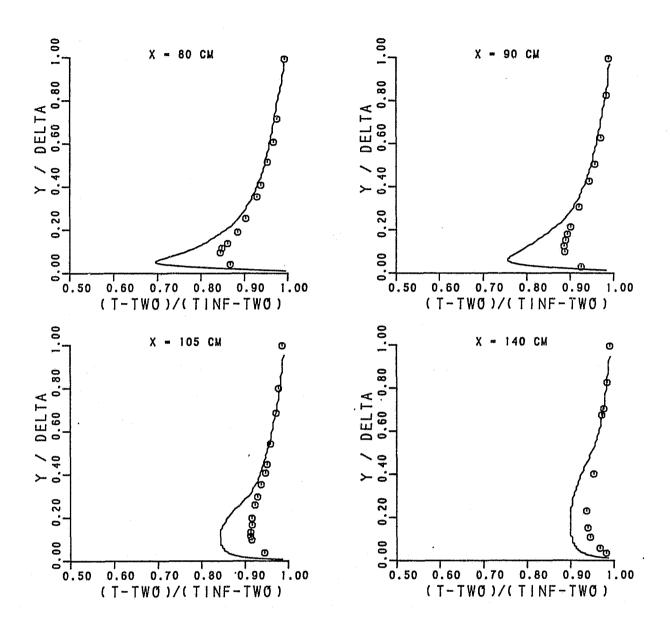


Figure 6.9-5. ASM Predictions of Mean Temperature Profile.

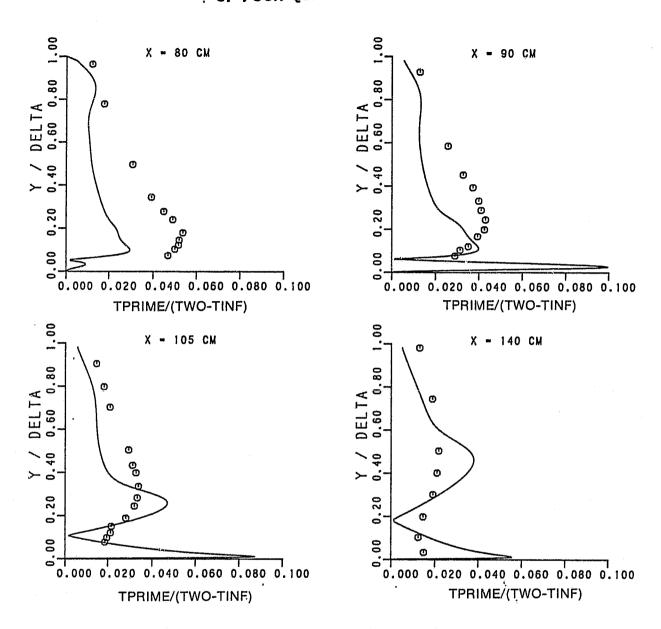


Figure 6.9-6. ASM Predictions of RMS Temperature Profile.

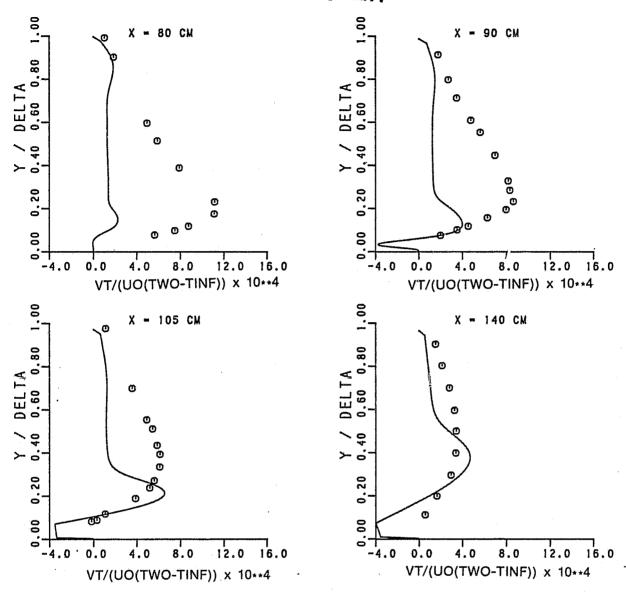


Figure 6.9-7. ASM Predictions of (vT').

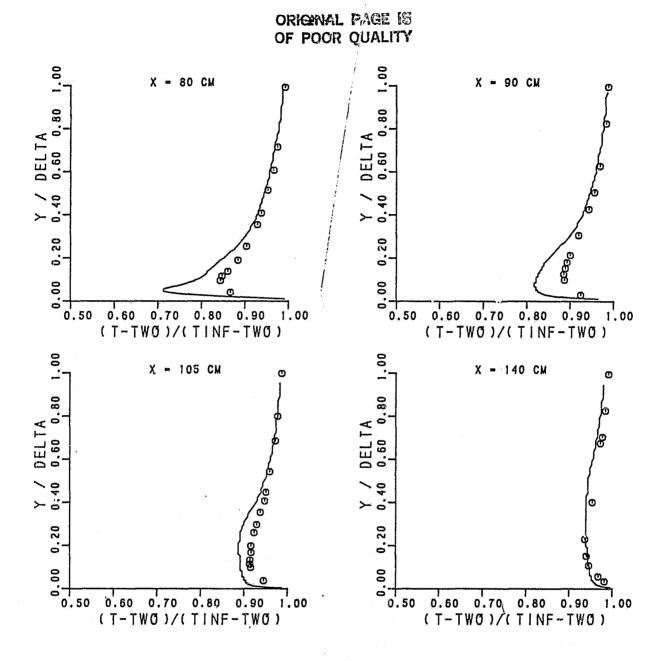


Figure 6.9-8. ASTM Predictions of Mean Temperature Profiles.

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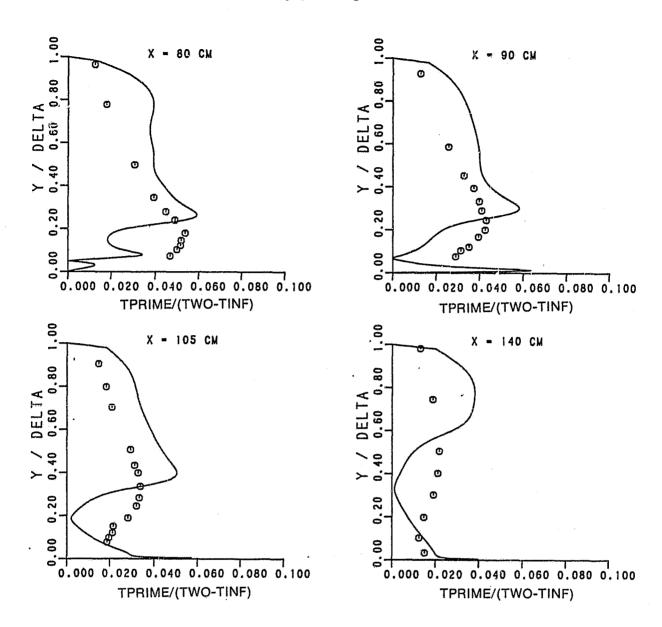


Figure 6.9-9. ASTM Predictions of the RMS Temperature Profile.

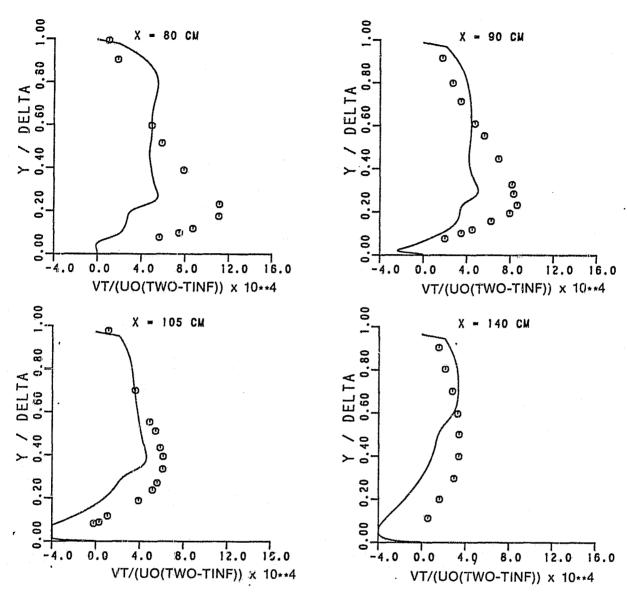


Figure 6.9-10. ASTM Predictions of $(\overline{vT'})$ Profiles.

6.10 Plug Flow Reactor

In reacting flows, the validation of the kinetic scheme is as important as the turbulence/chemistry interaction model. To validate the kinetic scheme, computations were made for the plug flow reactor shown schematically in Figure 6.10-1.

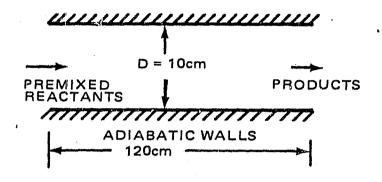
Measurements in a plug flow reactor were conducted by Hautman, et al., ¹⁹ for lean, stoichiometric, and rich propane flames. These measurements were used to test the validity of the four-step scheme that has been proposed by Glassman and his associates based upon detailed species and temperature measurements under a well-controlled low-pressure and high inlet temperature environment. The Glassman four-step scheme has been incorporated into the Garrett Combustion Codes, both parabolic and elliptic.

Computations were performed for lean, stoichiometric, and rich propane flames with both the two-step and the four-step schemes. Comparisons of these results with the measurements are shown in Figure 6.10-2 for the case of lean mixture. From Figure 6.10-1, it is clear that the four-step scheme is far superior to the two-step scheme in predicting the salient features of hydrocarbon combustion in the Princeton reactor.

It should be noted that the four-step scheme as proposed by Glassman and his associates was based upon data from their plug flow reactor. This scheme probably represents a closer approximation to actual hydrocarbon oxidation processes in a high temperature environment than the simpler two-step scheme does. How four-step correlates other reacting flow situations, such as a laminar diffusion flame, premixed turbulent flames, and jet flames, is covered in Paragraphs 6.11, 6.12 and 6.13, respectively.

HAUTMAN ET AL

PLUG FLOW REACTOR



U = 10.3485 M/S EQUIVALENCE RATIO = 0.12 T = 1021°K P = 1 ATM

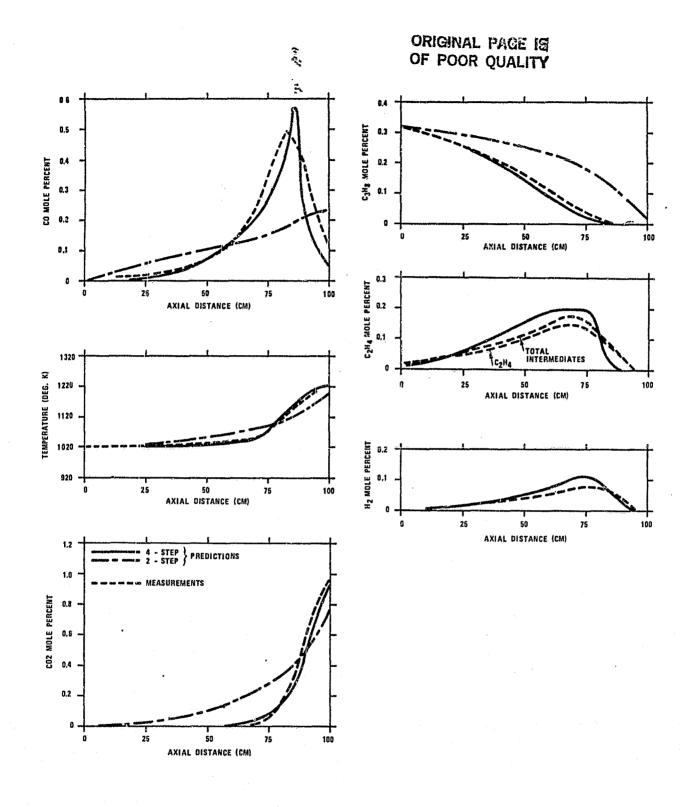


Figure 6.10-2. Comparison of 2-Step and 4-Step Kinetic Scheme With Lean Propane Premixed Flame Data From High Temperature Plug Flow Reactor.

6.11 Laminar Diffusion Flame

Another benchmark test case selected for validating the kinetic schemes is the laminar diffusion flame. Measurements for a laminar diffusion flame have been reported by Mitchell, et al. 129 for the setup shown in Figure 6.11-1. This flow was computed with the 2-D elliptic CPM. Runs of this type are useful in the validation of reaction mechanisms and establishing rate constant values since uncertainties due to turbulent interactions are absent.

Comparisons between the measured and predicted species concentration, temperature, and velocity at different axial locations are shown in Figures 6.11-2 through 6.11-8, respectively, at three axial stations. The predictions were obtained with both kinetic schemes and include the influence of buoyancy and variable thermodynamic and transport properties. Overall, the agreement between the predictions and measurements is fairly good.

Results with the two-step scheme for the first axial station (x = 1.2 cm) are presented in Figures 6.11-2 through 6.11-4. The overall heat release rate as indicated by axial velocity (V) correlation is in 900d agreement with data. Stable species profiles (e.g. CO_2 , H_2O , O_2 and unburned fuel) are also well correlated. The CO levels are predicted to be significantly lower than measurements by a factor of two to three. This is consistent with the two-step results on the plug flow reactor. Similar observation can be made for the comparison shown in Figures 6.11-5 and 6.11-6 at x = 2.4 cm. The temperature is slightly overpredicted (perhaps due to neglect of radiation losses in calculations) at x = 5 cm. The new CO prediction correlates well with the data.

The overall agreement between the two-step predictions and data is reasonable. The slight discrepancies are due to the following:

- (a) The presence of H_2 and intermediate hydrocarbons has been ignored in the two-step scheme. This results in overprediction of H_2O , CH_4 , and temperature. Some of these differences can be overcome with an improved scheme.
- (b) Differential diffusion of species has been ignored. This will be significant for ${\rm H_2}$ diffusion due to its low molecular weight.
- (c) Radiation was not considered in these computations.

The four-step results with the rate constants suggested by Hautman et al. are presented in Figures 6.11-9 through 6.11-15. Except for the velocity profile at x=1.2 cm, the scheme indicates good comparison with data as shown in Figure 6.11-9. The general shape of the temperature profile is well predicted as shown in Figure 6.11-10. Near the flame centerline at x=1.2 cm, the model underpredicts temperature levels by approximately 50 percent. The agreement improves further downstream, and by x=5 cm, the comparison is good. The fuel breakdown near the center is underpredicted by a factor of two as shown in Figure 6.11-11 for both x=1.2 and 2.4 cm. Similarly, for the initial portion of the flame, the CO_2 levels near the center are considerably different from data. The same is true of the other stable species; for example, O_2 and O_2 0 as shown in Figures 6.11-14 and 6.11-15.

The four-step predictions in regard to CO are considerably better than the two-step results shown in Figure 6.11-4 through 6.11-8. As shown in Figure 6.11-13, the CO peaks are similar in magnitude, as the data shows. Some improvement is desirable for the radial profile shape. Overall, the four-step correlates well with the data. Deficiencies are in regard to correlation in the initial portion of the flame centerline where the model underpredicts fuel breakdown and the levels of temperature, ${\rm CO_2}$, ${\rm CO_2}$ and ${\rm H_2O_2}$.

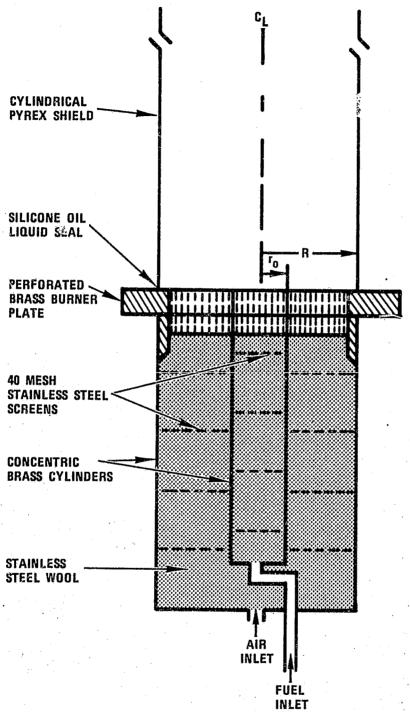


Figure 6.11-1. Schematic of Laminar Diffusion Flame Setup Used By Mitchell.

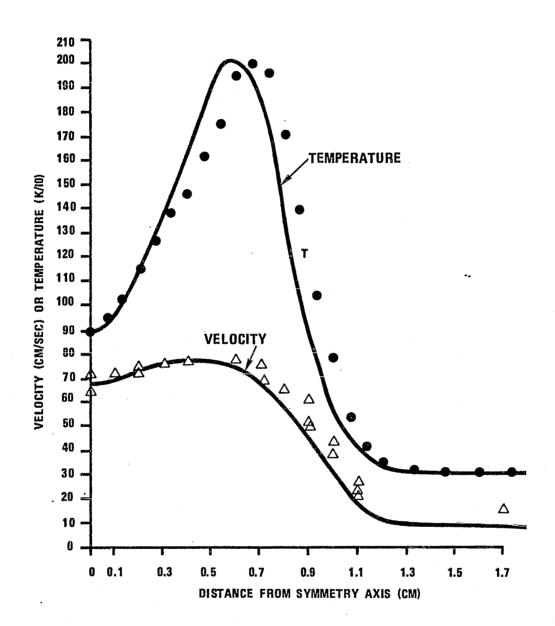


Figure 6.11.2. Comparison Between Two-Step Model Predictions and Measurements for Axial Velocity and Temperature Profiles of the Mitchell's Laminar Diffusion Flame at 1.2 cm Above the Burner Plate.

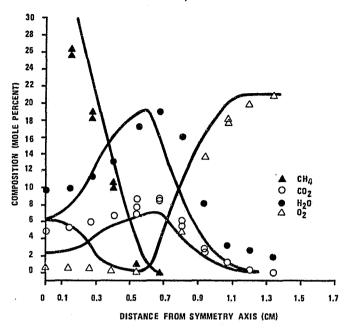


Figure 6.11-3. Two-Step Predictions and Measurements for CH_4 , CO_2 , H_2O and O_2 Profiles, X = 1.2 cm.

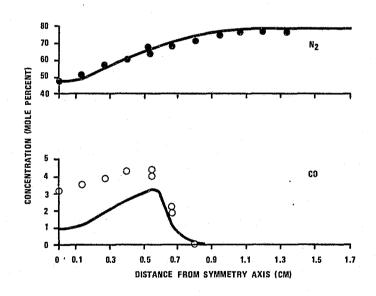


Figure 6.11-4. Two-Step Predictions and Measurements for N_2 and CO Profiles, X = 1.2 cm.

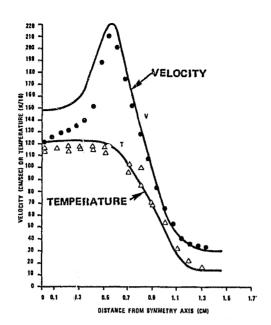


Figure 6.11-5. Comparison Between Two-Step Predictions and Measurements of Velocity and Temperature Profiles of the Mitchell's Laminar Diffusion Flame at x = 2.4 cm.

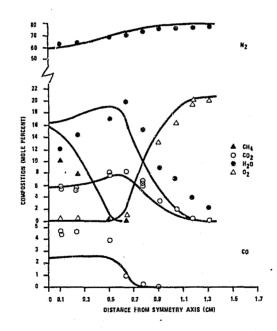


Figure 6.11-6. Predicted and Measured Species Profiles at X = 2.4 cm. (Two-Step)

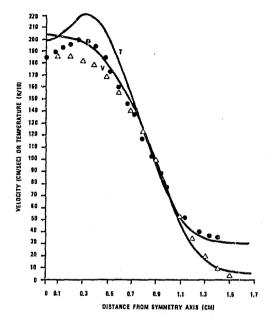


Figure 6.11-7. Comparison Between Predicted and Measured Axial Velocity and Temperature Profiles and Mitchell's Laminar Diffusion Flame at X = 5.0 cm. (Two-Step)

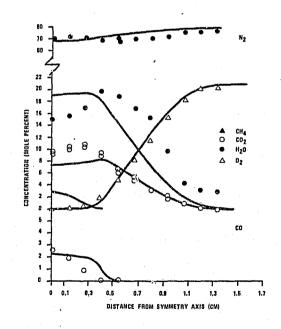
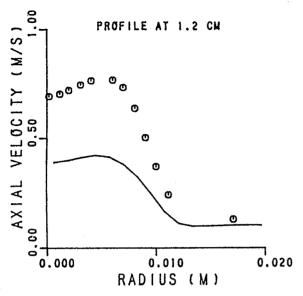
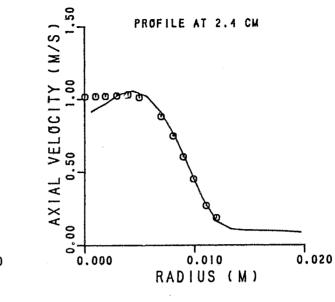


Figure 6.11-8. Predicted and Measured Species Profiles at X = 5.0 cm. (Two-Step)





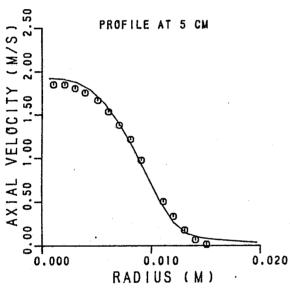


Figure 6.11-9. 4-Step Scheme, Axial Velocity Profiles.

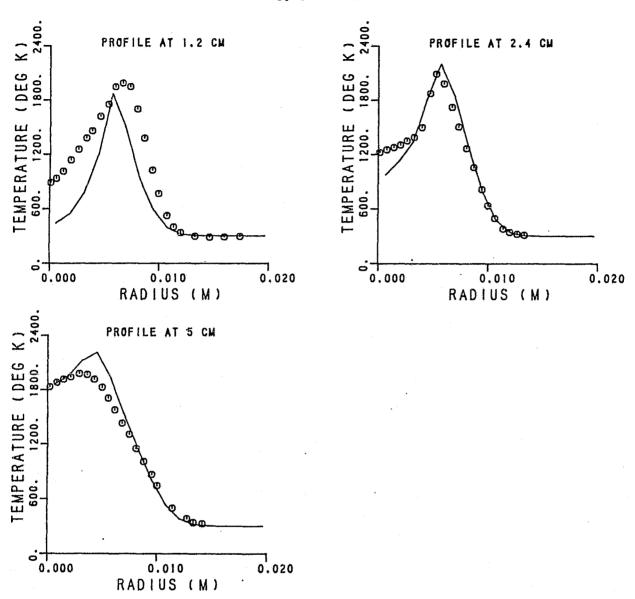
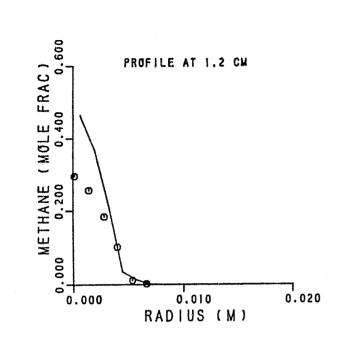


Figure 6.11-10. 4-Step Scheme, Temperature Profiles



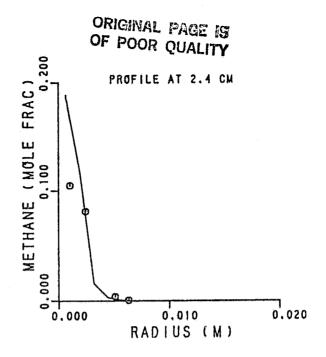
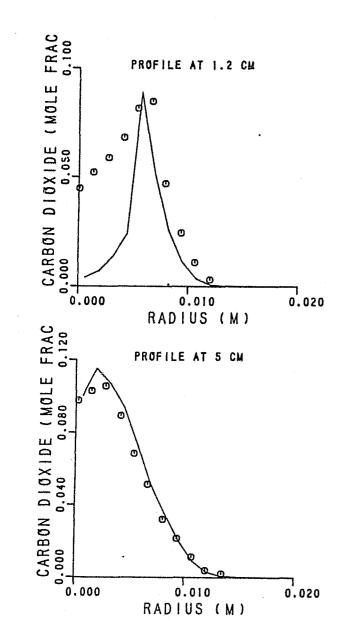


Figure 6.11-11. 4-Step Scheme, Methane Profiles.



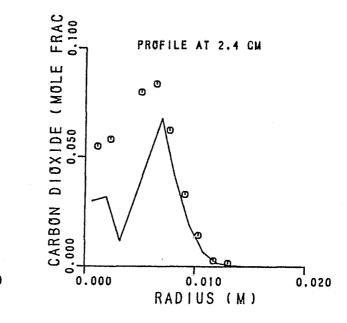
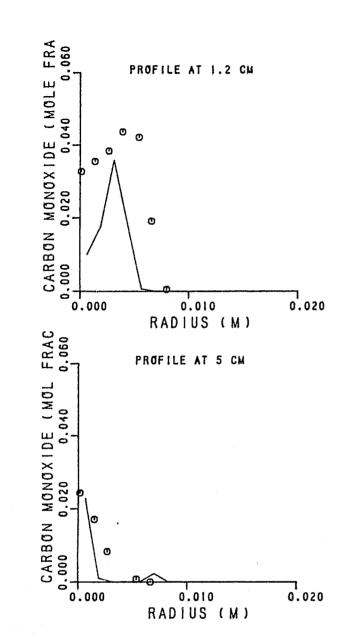


Figure 6.11-12. 4-Step Scheme, CO2 Profiles.



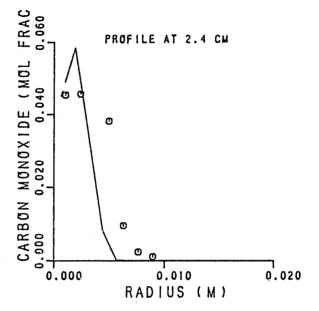


Figure 6.11-13. 4-Step Scheme, CO Profiles.

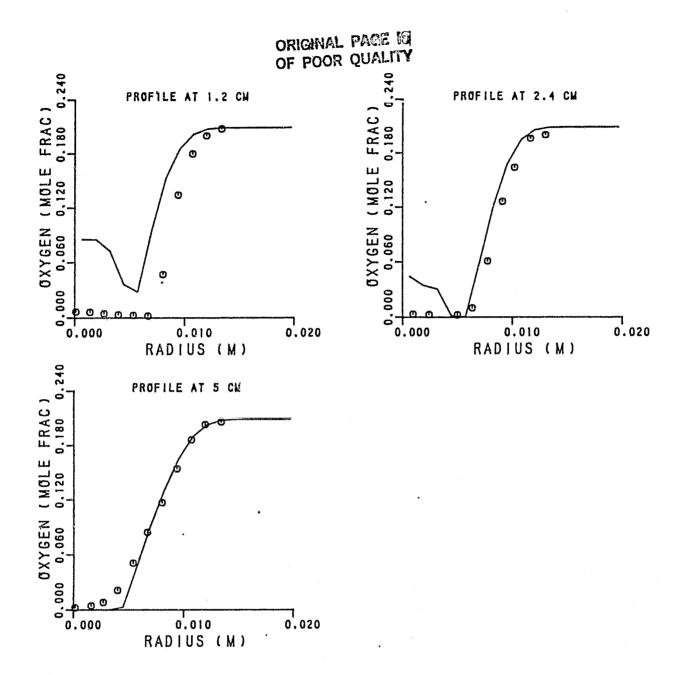


Figure 6.11-14. 4-Step Scheme, O2 Profiles.

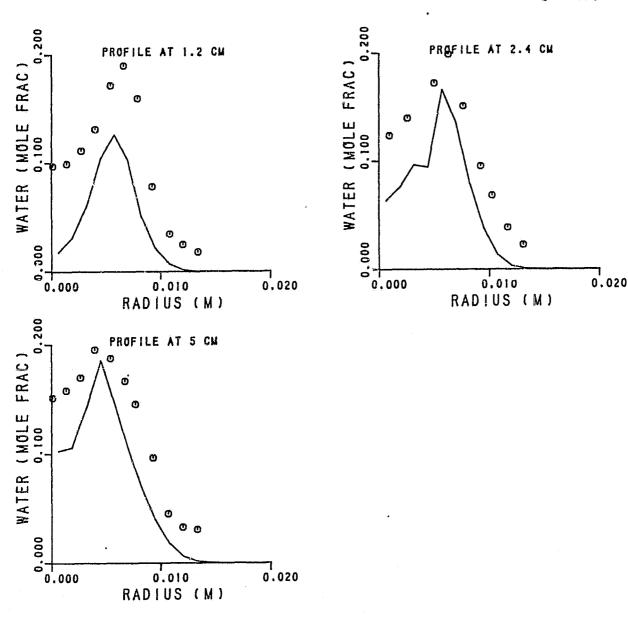


Figure 6.11-15. 4-Step Scheme, H₂O Profiles

6.12 Turbulent Premixed Flame in a Rectangular Duct

Another test case selected from the data base for evaluating kinetic schemes is the reacting flow of premixed propane/air in a rectangular duct with a flame stabilizer as shown in Figure 6.12-1. Measurements for this flow were made by Shipman, 137, 138 et al.

Computations for this case were performed using the 2-D parabolic program and standard k-& model, with the initial profiles obtained from measurements 0.0508 m downstream of the flame holder. The average inlet velocity was 18.288 m/s at a pressure of one atmosphere, having a turbulence intensity of 3 percent. Along the plane of symmetry, a zero radial gradient was specified for all the variables except V, which was set to zero. Along the outer radial boundary, wall function treatment was employed. Computations were performed with two-step and four-step kinetic schemes. On the two-step scheme, two different sets of rate constants were used. One of them corresponds with the constants established in the Army Combustor Design Criteria Program, and the other set is for the PM/PV combustion. Table 14 provides the values of the Arrhenius pre-exponents and the activation temperatures for the reaction steps.

TABLE 14. TWO-STEP RATE CONSTANTS FOR GARRETT/AVLABS AND PREMIXED/PREVAPORIZING REACTION.

	REACTION STEP 1		REACTION STEP 2	
	Pre-	Activation	Pre-	Activation
	Exponent	Temperature	Exponent	Temperature
Design Criteria	3.3×10^{14} 3.9×10^{9}	27,000	6.0x10 ⁸	12,500
PM/PV		18,000	2.2x10 ⁸	12,500

The predictions obtained using the Design Criteria constants are shown in Figures 6.12-2 through 6.12-8, and those using the PM/PV constants are presented in Figures 6.12-9 through 6.12-15.

The predicted mean axial velocity using the Design Criteria constant and the measurements are shown in Figure 6.12-2 at five

axial stations downstream of the flame holder. The predicted axial velocity profiles show slower mixing rates compared to the measurements. The velocities near the plane of symmetry are considerably smaller in the predictions than in the data.

Figure 6.12-3 illustrates the computed profiles of unburned fuel and data at five axial stations. The predicted unburned fuel mass fractions are higher than the measured values indicating slower fuel disappearance rate. Figure 6.12-4 illustrates the comparison between predicted and measured CO mass fraction. The predicted CO profiles are significantly lower than the data up to x = 0.2032, partly due to the slow reaction rates. Beyond this station, the CO mass fractions are in reasonable agreement with data. However, the radial spread of CO profiles are underpredicted by the model.

Since the reaction rates are underpredicted by the design criteria rate constants, the predicted temperatures (Figure 6.12-5) are also lower than the measurements. The radial spreading of temperature profile is also underpredicted by the model.

The other derived variables such as O_2 , CO_2 and $\mathrm{H}_2\mathrm{O}$ are presented in Figures 6.12-6 through 6.12-8, respectively. Due to the lower fuel consumption rate, predicted O_2 profiles are higher than measurements. Similarly the discrepancy between predictions and measured CO_2 can be explained. Apparent improvement in regard to $\mathrm{H}_2\mathrm{O}$ profiles may be due to faster diffusion rates of this species compared to model assumptions of equal diffusivity for all species.

In conclusion, the Army Combustor Design Criteria rate constants appear to underpredict fuel consumption rate and temperature profiles. On occasions the design criteria constants have seemed to overpredict reaction rates. More extensive validation is needed to establish the two-step rate constants for both diffusion and premixed flames.

The predicted results for mean velocity, obtained by using the PM/PV rate constants, are presented in Figure 6.12-9. A substantial improvement can be observed in the agreement between data and predictions, when compared to the results using Design Criteria rate constants (Figure 6.12-2). This is due to faster fuel consumption. Figure 6.12-10 illustrates the comparison of data and predictions for unburned fuel. These profiles are in much better agreement than the results obtained from the first set of rate constants. However, the radial diffusion rates are still underpredicted by the model.

The comparison between predicted and measured ${\rm CO_2}$ profiles are presented in Figure 6.12-11. Due to the improved convection rates, the reaction rates are expected to be higher, and hence the ${\rm CO_2}$ values are higher than the values obtained from the design criteria rate constants. The ${\rm CO_2}$ values predicted from the PM/PV rate constants are still smaller than the measured values.

The predicted and increased profiles for CO are illustrated in Figure 6.12-12. The predicted peak CO values are higher than the data and the predicted CO mass fraction profiles do not spread radially outwards as much as seen in the measurements.

The predicted temperature distributions using the PM/PV rate constants and the measurements are presented in Figure 6.12-13. Since the reaction rates are faster, it is expected that the predicted temperatures are also higher than those obtained using the design criteria rate constants. Overall these profiles are in good agreement with data.

Figures 6.12-14 and 6.12-15 show comparisons between measured and predicted profiles of $\rm O_2$ and $\rm H_2O$, respectively. Although there is improvement over the design criteria constants in regard to $\rm O_2$

and ${\rm CO}_2$, the comparison is worse for ${\rm H}_2{\rm O}$. This may be due to a number of reasons, such as:

- O Incorrect approximation of fuel breakdown by simple twostep
- O Neglect of H₂ as one of the intermediate products
- O Assumption of equal diffusivities of all gaseous molecules
- o Turbulence/chemistry interaction represented by a simple eddy breakup model

Calculations were also performed using the four-step kinetic scheme outlined in Section 3.0. The rate constants used in this computation were obtained from the report of Hautman, 19 et al. These rate constants have given good comparison with plug flow reaction as shown in Figure 6.10-1. The Arrhenius pre-exponents and the activation temperatures for each of the four steps are given in Table 15.

TABLE 15. RATE CONSTANTS FOR 4-STEP KINETIC SCHEME.

REACTION STEP	ARRHENIUS PRE-EXPONENT (K _O)	ACTIVATION TEMPERATURE	EDDY BREAKUP CONSTANT (C _R)
1	2.0893 x 10 ²²	24,800	3.0
2	5.0117×10^{19}	25,000	3.0
3	3.9811 x 10 ¹⁹	20,000	3.0
4	3.3113 x 10 ¹⁸	20,500	3.0

The predicted mean axial velocity profiles using the four-step kinetic scheme and the data are presented in Figure 6.12-16. The predicted velocities are significantly smaller than the measurements. Predicted unburned fuel profiles are shown in Figure 6.12-17 along with the data. Comparison with the two-step results (Figure 6.12-14) shows that there are no appreciable differences in the unburned fuel profiles between four-step and two-step.

The four-step predictions for CO are presented in Figure 6.12-18. Due to the slow reaction rates in the four-step scheme, the predicted CO values are smaller compared to both the data and the two-step scheme (Figures 6.12-4 and 6.12-12). Consequently, as shown in Figure 6.12-19 the four-step predicted temperature profiles are lower than the two-step (Figures 6.12-5 and 6.12-13) and the data. The other derived variables are similar including O_2 , O_2 and O_2 0 shown in Figures 6.12-20 through 6.12-22.

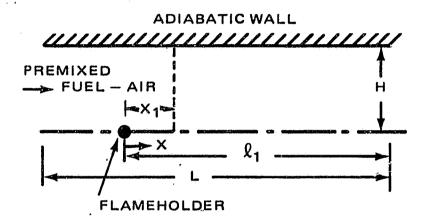
A number of reasons can be forwarded for delivering poor correlation with the four-step scheme. Numerical experimentation was made to demonstrate that the basic mechanism is valid and that future modifications to the approach will yield good comparison. Figures 6.12-23 through 6.12-29 present results with the first two reaction-step rate constants changed

$$K_{O_1} = 2.0893 \times 10^{24}$$
 $C_{R_1} = 6.0$
 $K_{O_2} = 5.0117 \times 10^{21}$ $C_{R_2} = 6.0$

Significant improvement in predictions can be seen, and one can therefore conclude that the basic four-step hydrocarbon oxidation mechanism is valid.

SHIPMAN AND CO-WORKERS

CONFINED STOICHIOMETRIC FLAME STABILIZED ON A CYLINDRICAL FLAMEHOLDER IN A RECTANGULAR DUCT



DUCT WIDTH = 0.0254 M

H = 0.0381 M

 $X_1 = 0.0508 M$

 $\ell_1 = 0.3080 \text{ M}$

L = 0.4286 M

 \mathbf{X}_1 denotes first measurement location from which calculations are started.

AVERAGE U = 18.288 M/S

• P = 1 ATM

Figure 6.12-1. Geometry of Turbulent Premixed Flame in a Rectangular Duct.

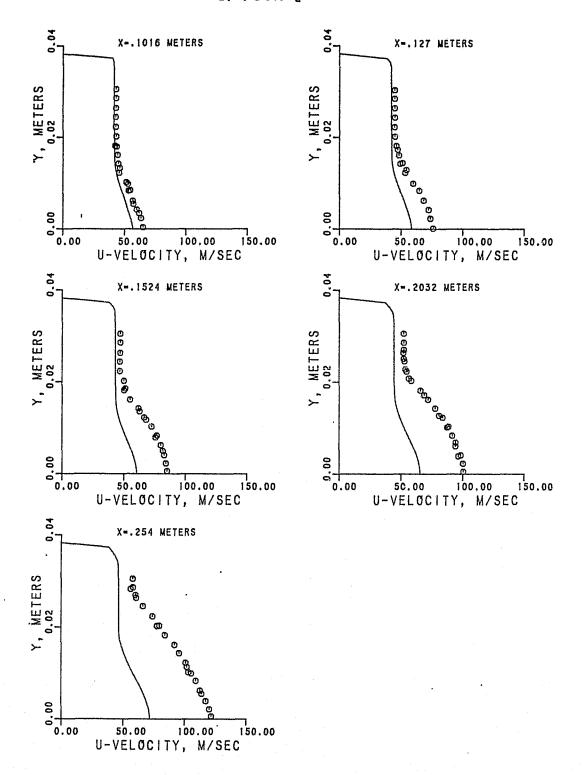


Figure 6.12-2. Predicted Velocity Profiles With Design Criteria Rate Constants.

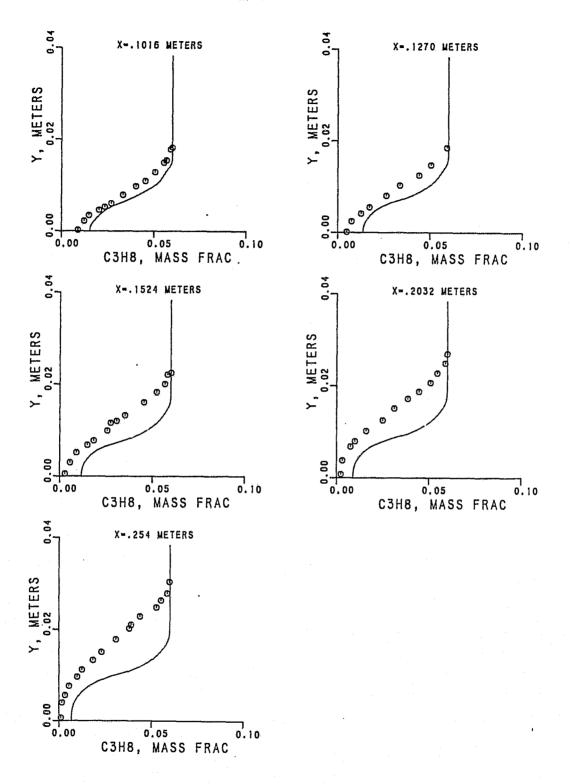


Figure 6.12-3. Predicted Unburned Fuel Profiles With Design Criteria Rate Constants.

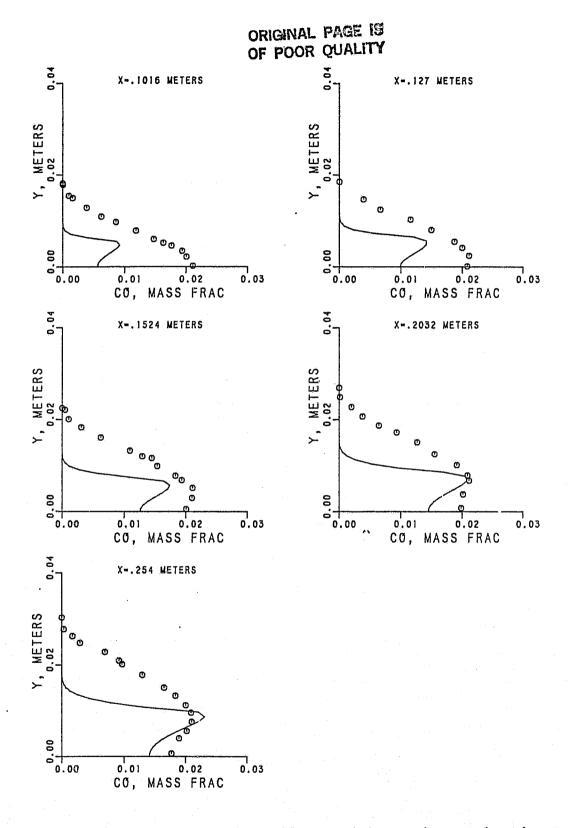


Figure 6.12-4. Predicted CO Profiles With Design Criteria Rate Constants.

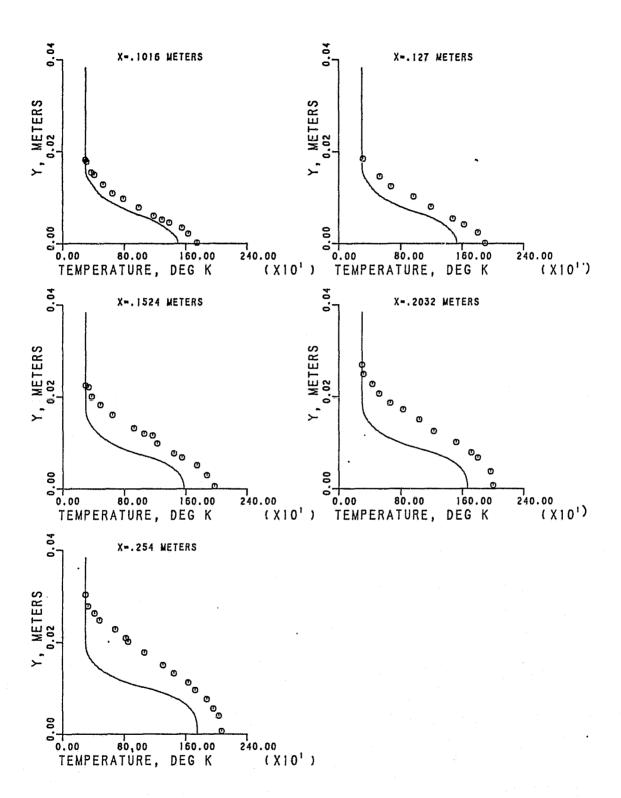


Figure 6.12-5. Predicted Temperature Profiles With Design Criteria Rate Constants.

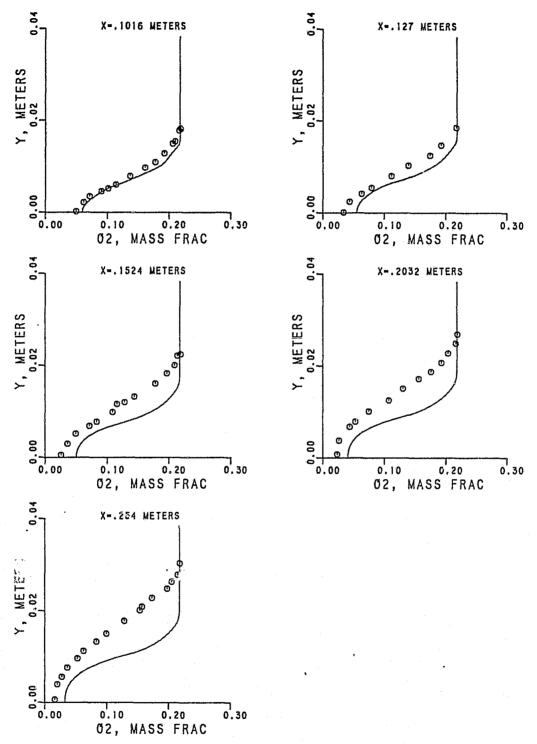


Figure 6.12-6. Predicted O_2 Mass Fraction With Design Criteria Rate Constants.

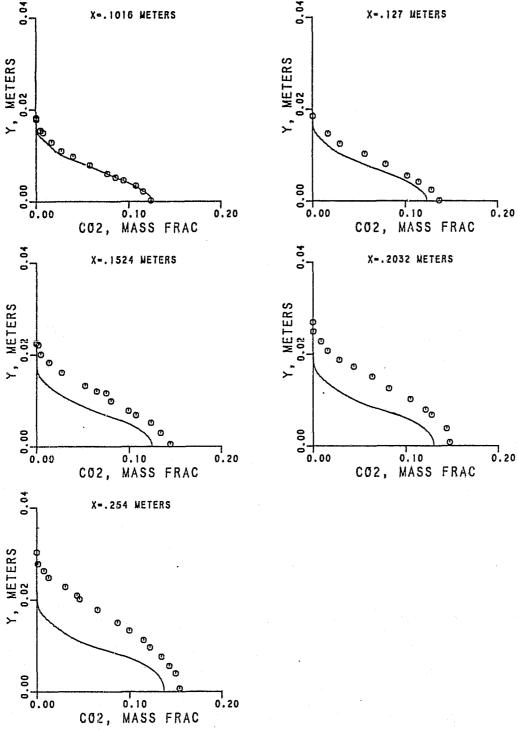


Figure 6.12-7. Predicted CO₂ Profiles With Design Criteria Rate Constants.

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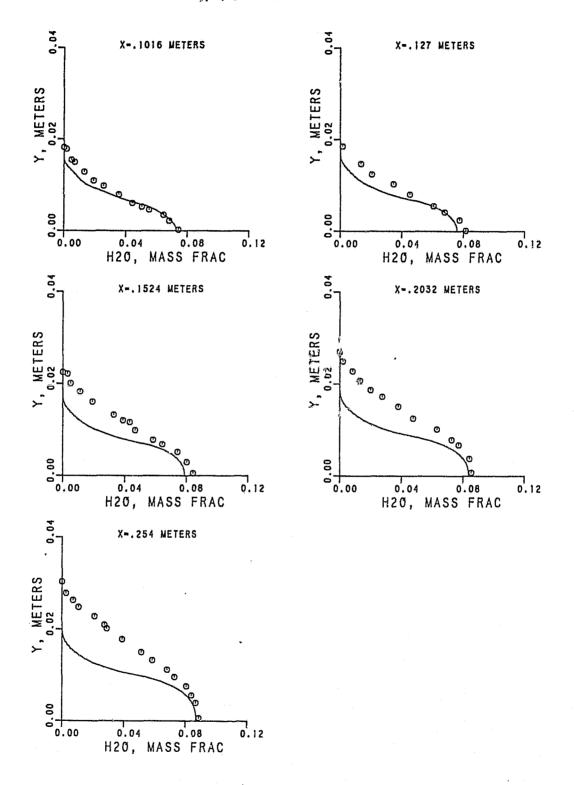


Figure 6.12-8. Predicted H₂O Profiles With Design Criteria Rate Constants.

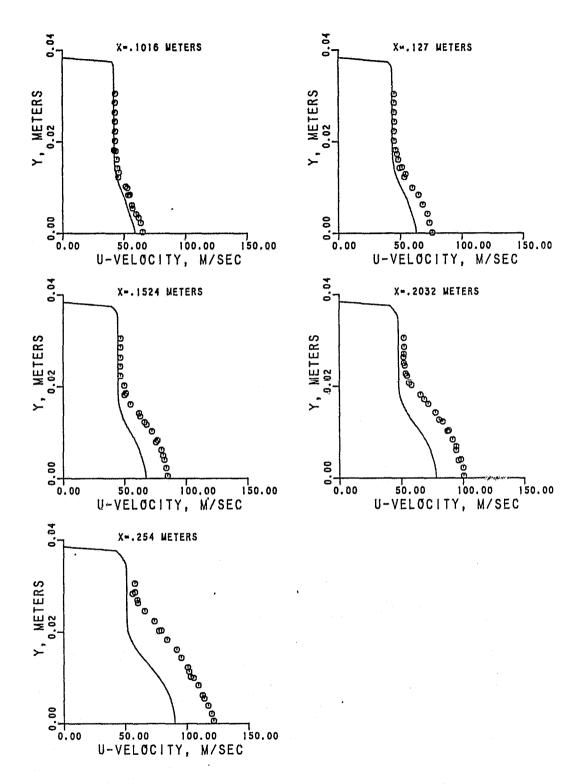


Figure 6.12-9. Predicted Velocity Profiles With PM/PV Rate Constants.

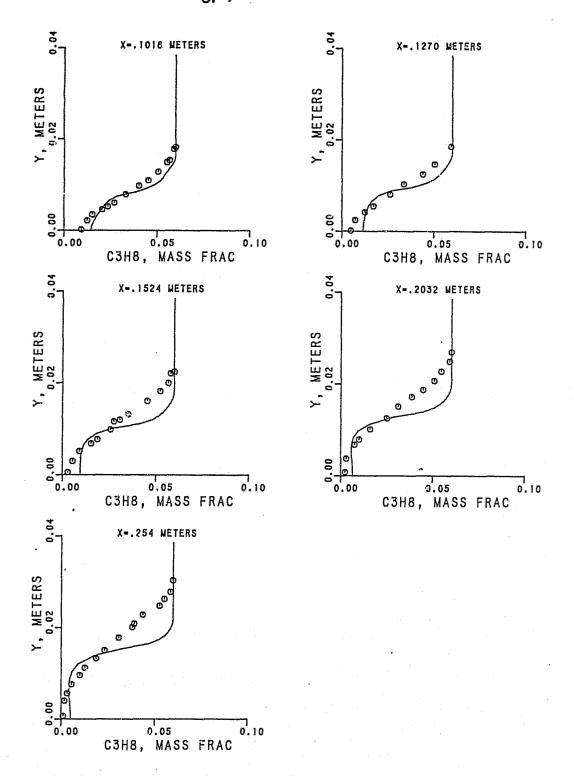


Figure 6.12-10. Predicted Unburned Fuel Profiles With PM/PV Rate Constants.

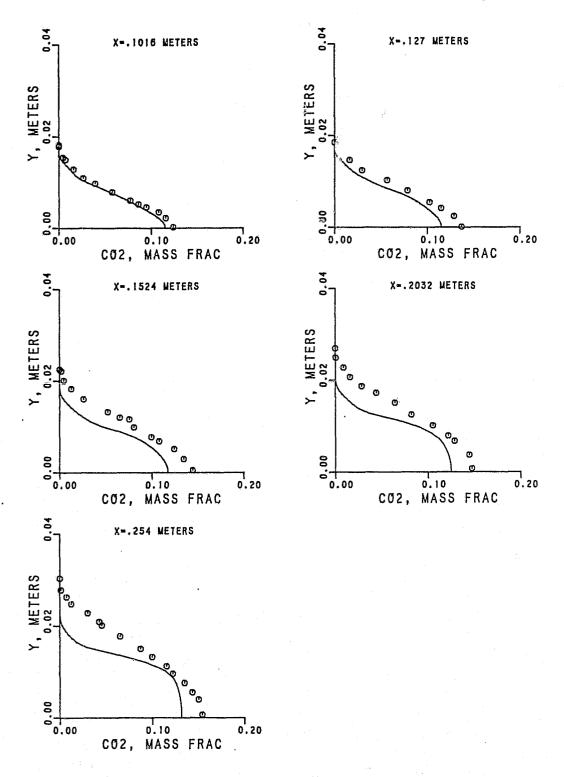


Figure 6.12-11. Predicted ${\rm CO}_2$ Profiles With PM/PV Rate Constants.

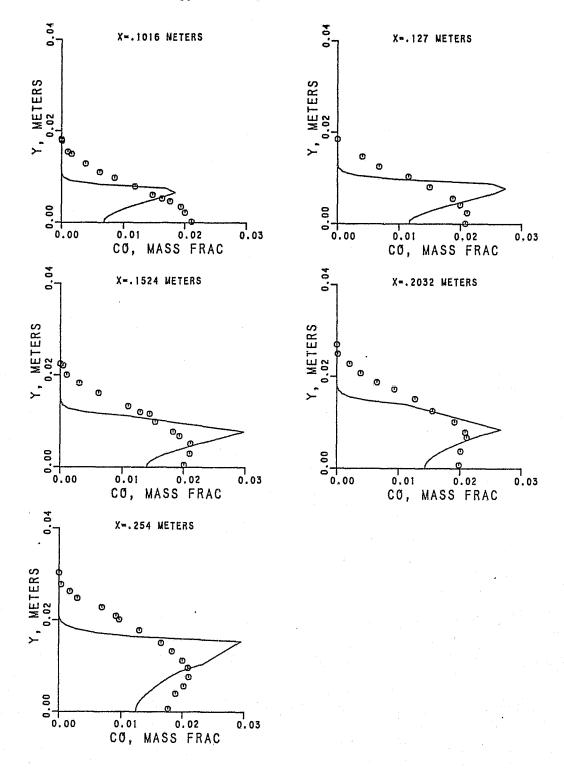


Figure 6.12-12. Predicted CO Profiles With PM/PV Rate Constants.

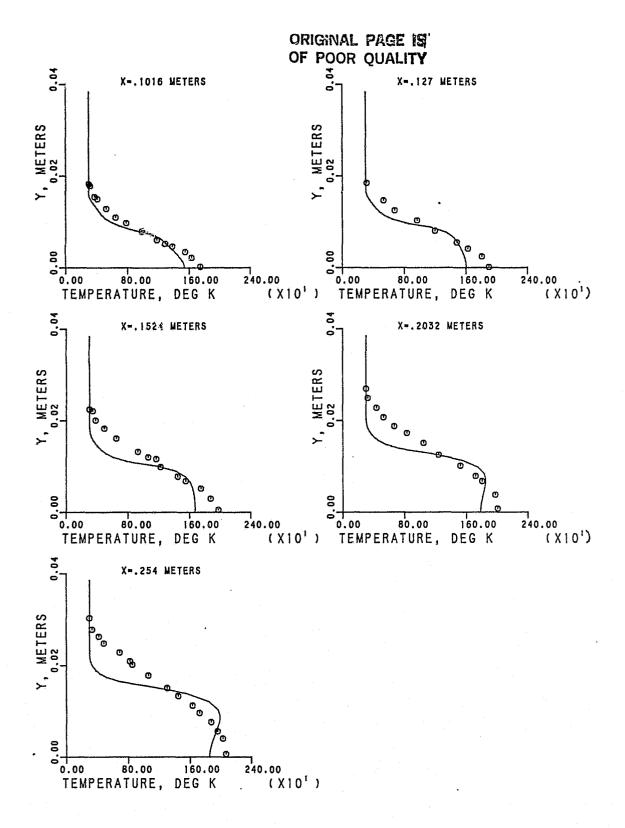


Figure 6.12-13. Predicted Temperature Profiles With PM/PV Rate Constants.

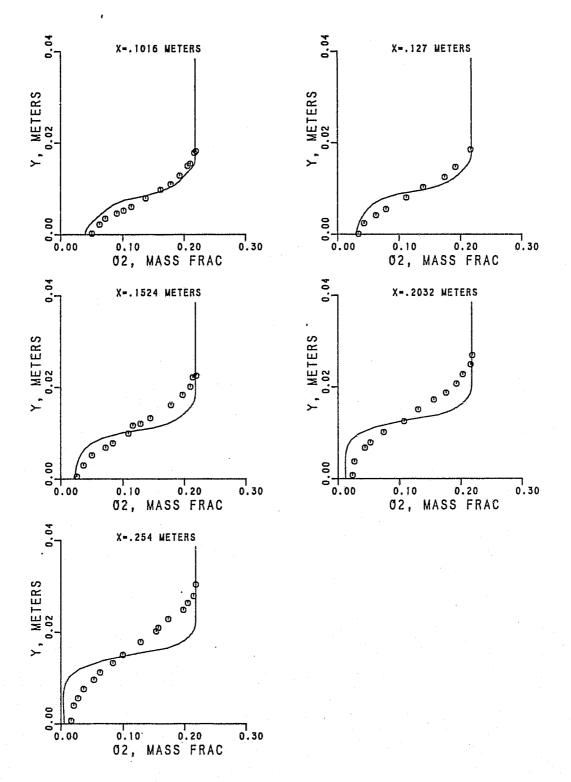


Figure 6.12-14. Predicted O₂ Profiles With PM/PV Rate Constants.

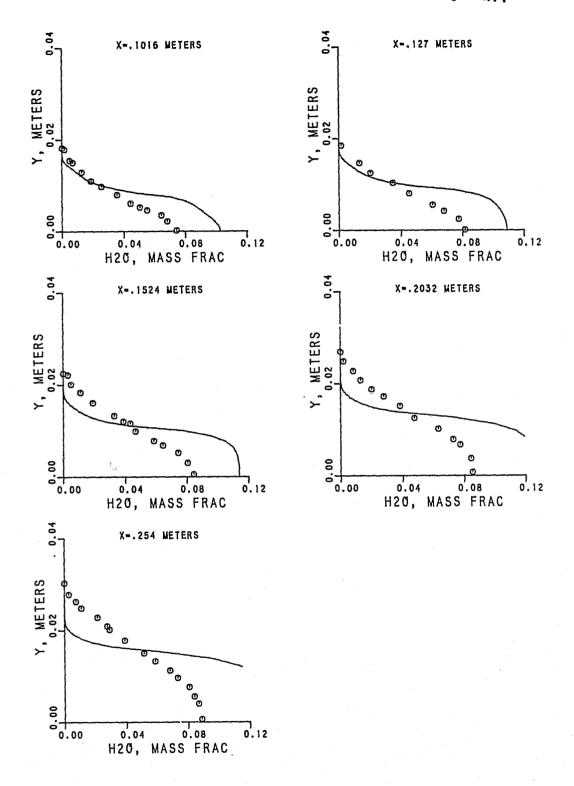


Figure 6.12-15. Predicted H_2O Profiles With PM/PV Rate Constants.

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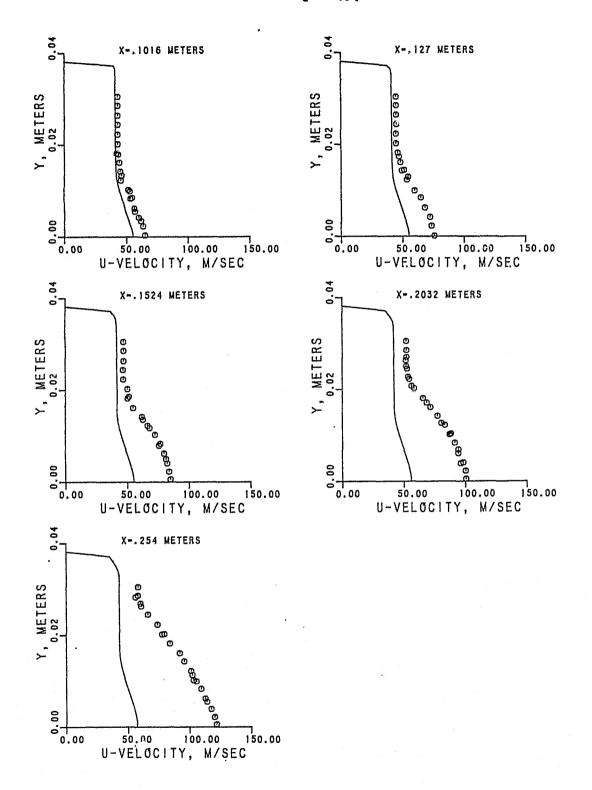


Figure 6.12-16. Predicted Velocity Profiles With The 4-Step Scheme.

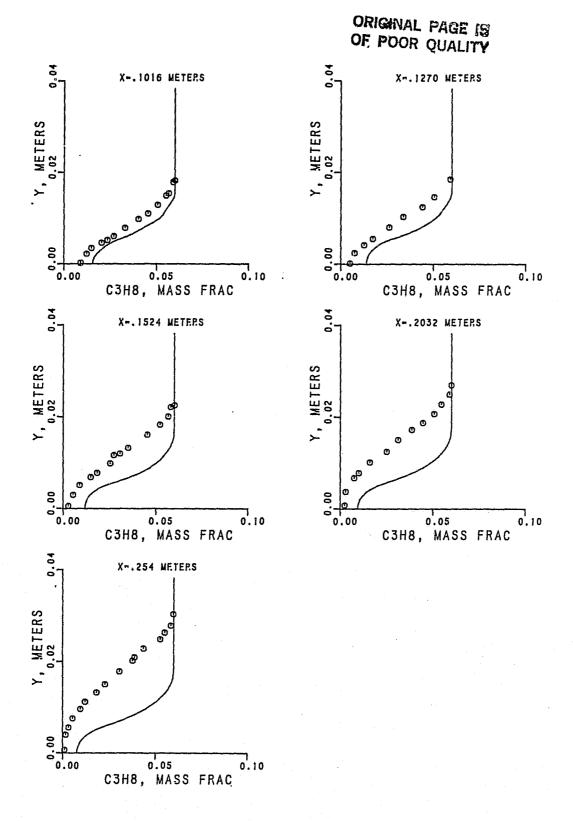


Figure 6.12-17. Predicted Unburned Fuel Profiles With The 4-Step Scheme.

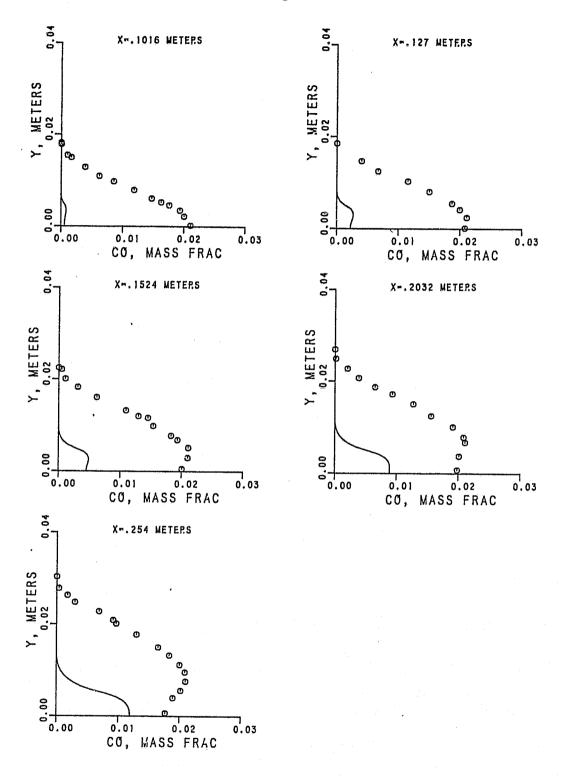


Figure 6.12-18. Predicted CO Profiles With The 4-Step Scheme.

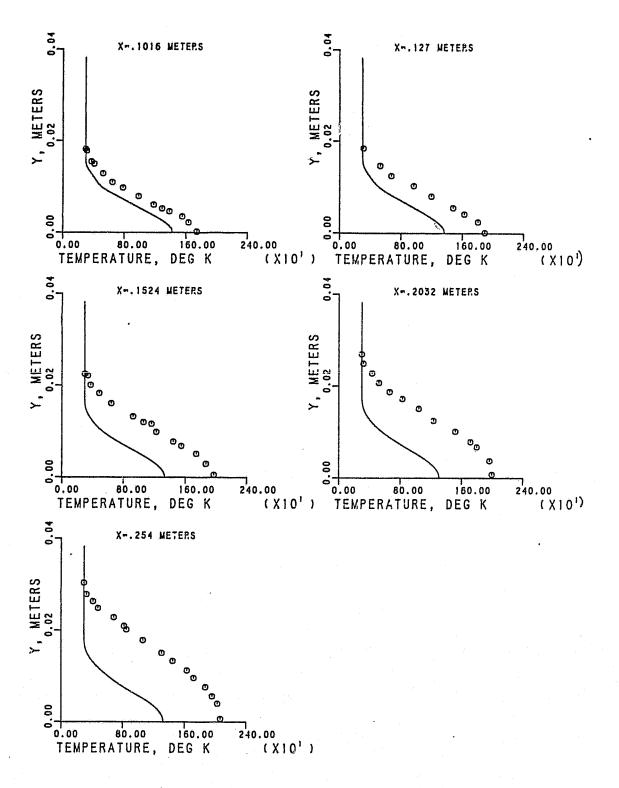


Figure 6.12-19. Predicted Temperature Profiles With The 4-Step Scheme.

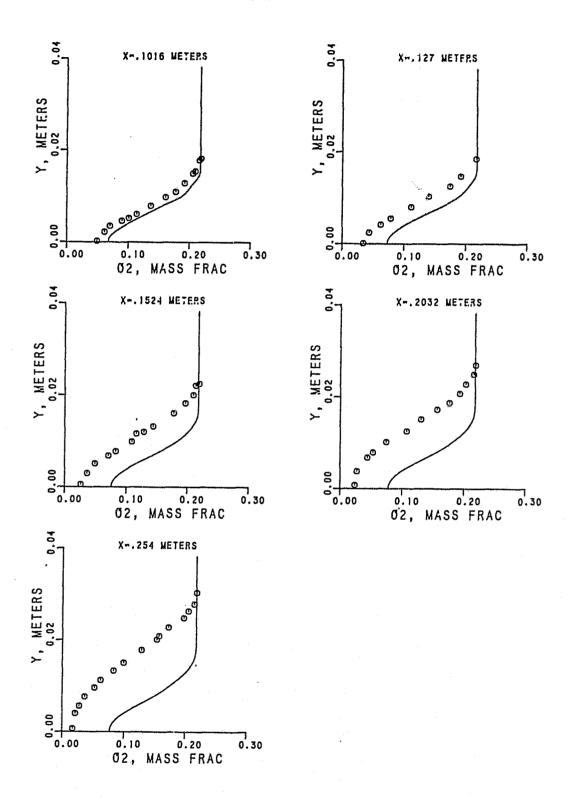


Figure 6.12-20. Predicted ${\rm O_2}$ Profiles With The 4-Step Scheme.

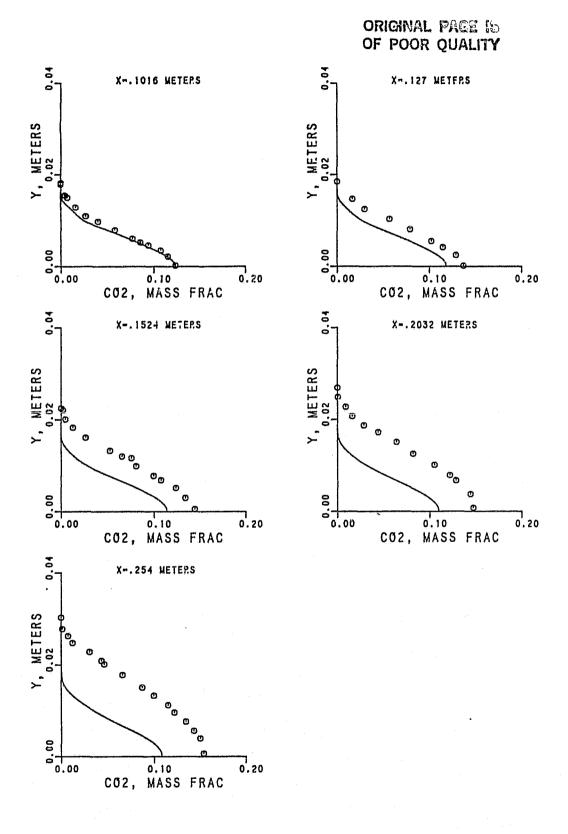


Figure 6.12-21. Predicted CO₂ Profiles With The 4-Step Scheme.

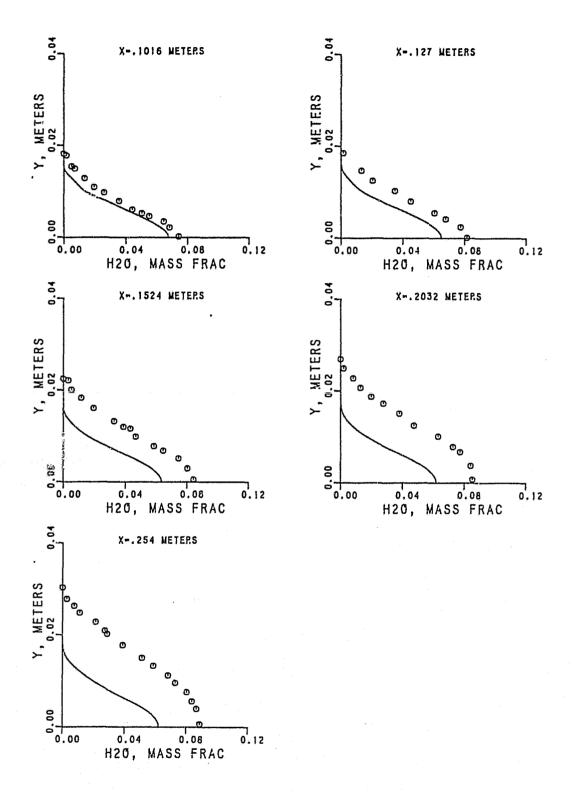


Figure 6.12-22. Predicted H_2O Profiles With The 4-Step Scheme. 280

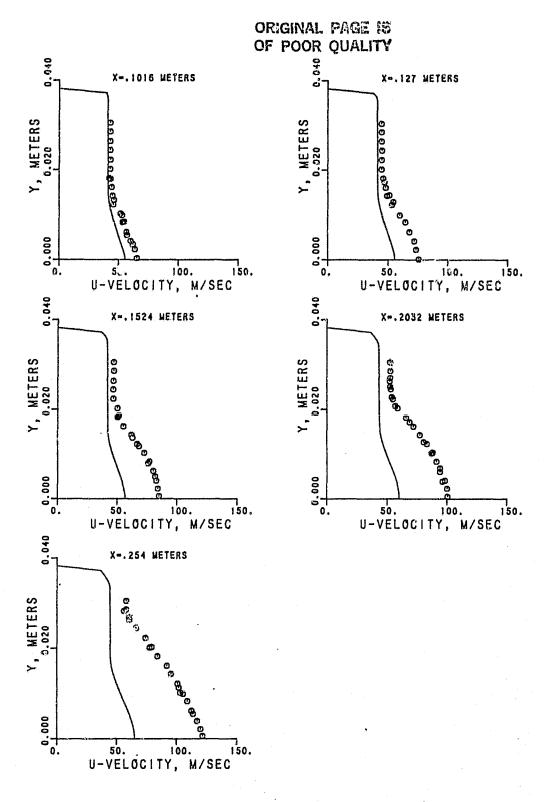


Figure 6.12-23. 4-Step Scheme With Modified Rate Constants For Fuel and Intermediate Fuel Reaction Steps (Modified 4-step) Axial Velocity Profile.

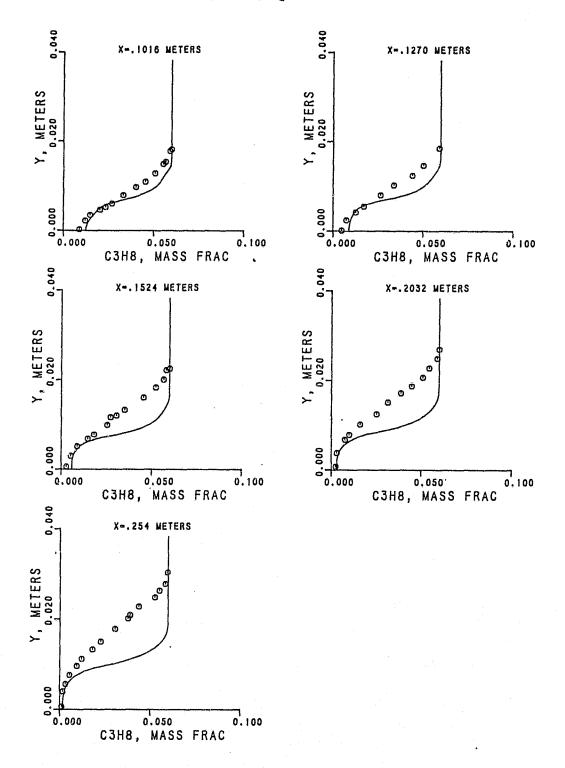


Figure 6.12-24. Modified 4-Step -- Unburned Fuel Profiles.

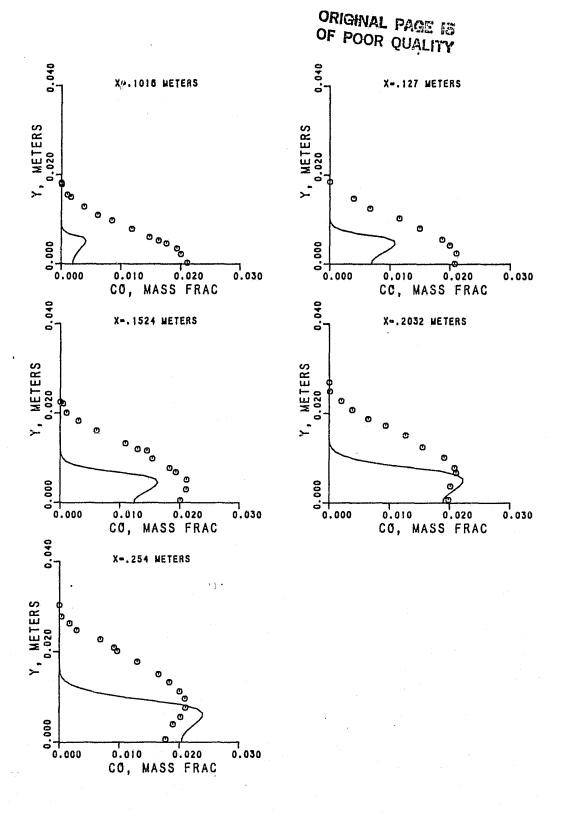


Figure 6.12-25. Modified 4-Step CO Profiles.

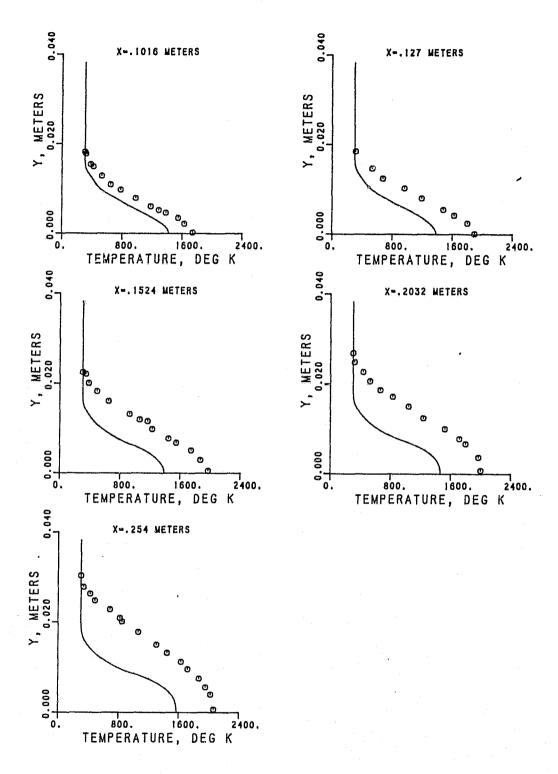


Figure 6.12-26. Modified 4-Step -- Temperature Profiles.

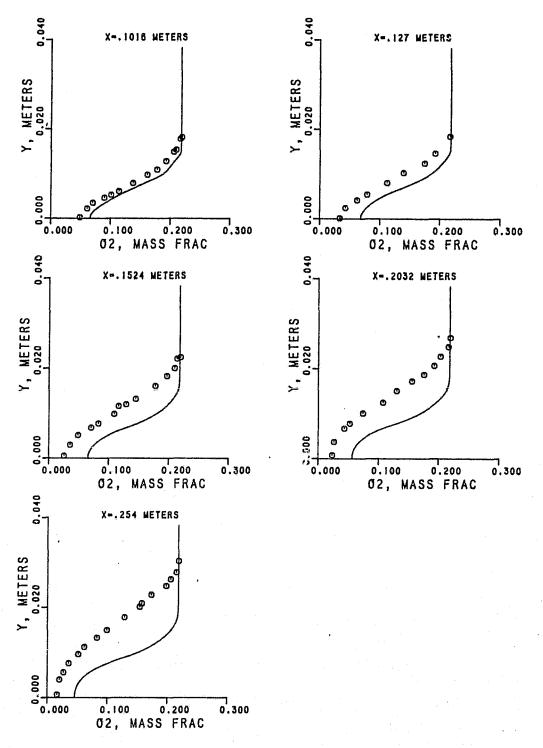


Figure 6.12-27. Modified 4-Step -- 02 Profiles.

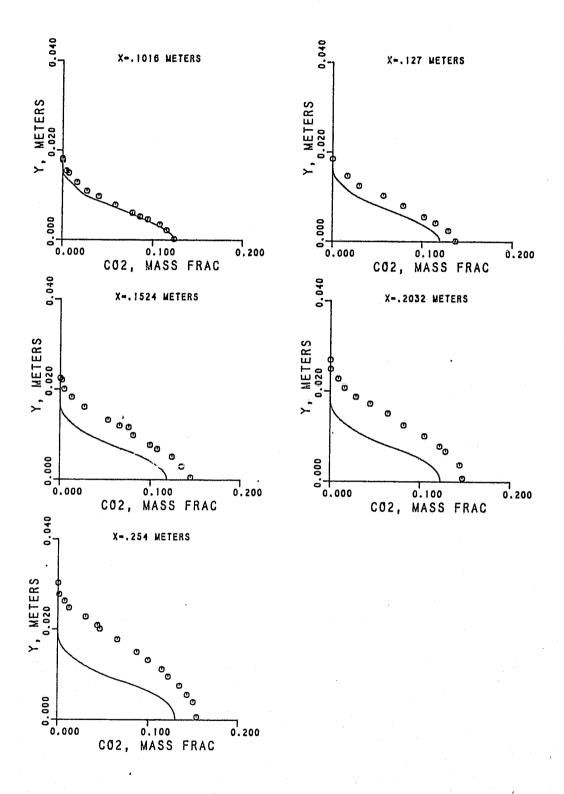


Figure 6.12-28. Modified 4-Step -- CO₂ Profiles.

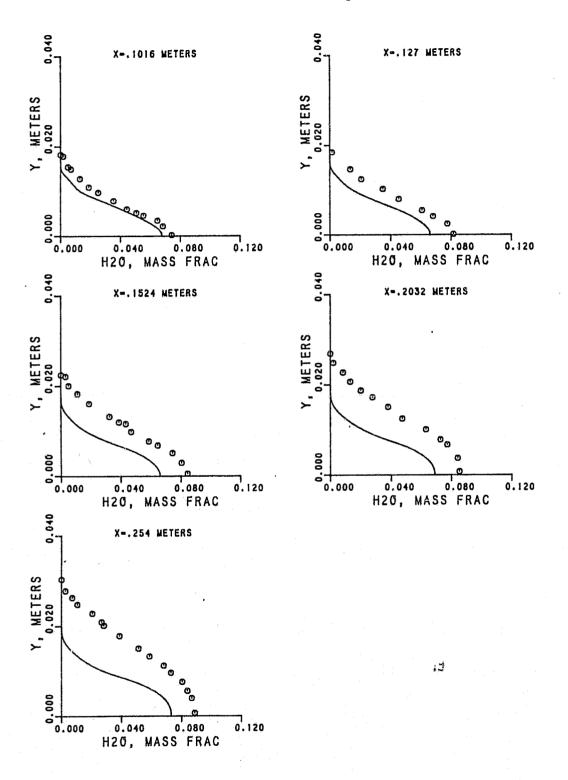


Figure 6.12-29. Modified 4-Step -- H2O Profiles.

6.13 Free Methane Turbulent Jet Flame

The free, turbulent, reacting methane jet investigated by Hassan, et al., 133 was modeled here using the PDF-partial equilibrium approach of Bilger and Starner. 27 Although several configurations were studied by Hassan, the detailed data was available only on the flame that has been investigated here. The test setup was a vertical free turbulent methane jet issuing from a 7.74 mm diameter pipe as shown schematically in Figure 6.13-1. The jet Reynolds number was 15,000, with a bulk velocity of 39.9 m/s. The flame was stabilized by a co-annular flow of 1 percent (by mass) of hydrogen. A discussion of the data and the results of the numerical model are presented below.

From the initial (or tube exit) jet velocity, mass flow and assumed temperature of 59°F, mass and energy flux can be determined for comparison at downstream positions. The fuel was reported to be 94 percent methane. From the assumption of atmospheric pressure and the reported density, a molecular weight of 17.22 was determined. If the remaining 6 percent was composed of nitrogen and propane (typical dry natural gas composition), then 52.4 percent of that fraction being nitrogen would give the above molecular weight. From the reported mass flows of H₂ and fuel, the following mole fractions were determined,

 X_{fuel} = 78.86%, X_{CH_4} = 74.13, X_{N_2} = 2.48, $X_{\text{C}_3\text{H}_8}$ = 2.25, X_{H_2} = 21.

The specific enthalpy at the jet exit is then $-4.154.10^6 \frac{J}{kg}$ and energy flux is $-5858 \frac{J}{sec}$.

At four axial positions (x/D = 36.2, 75, 113.7 and 204) radial profiles of temperature, mole fractions of CO, CO_2 and O_2 were reported. Consider the reaction equation in mole fraction form,

$$F C_{CX} H_{CY} N_{CN} + A (O_2 + \frac{N_2}{O_2} N_2) \rightarrow \chi_{CO} + \chi_{CO_2} + \chi_{O_2} + \chi_{CH_4} + \chi_{CH_2} + \chi_{H_2} + \chi_{H_2O} + \chi_{N_2}$$

Although dry measurements were made, the following analysis assumes that the reported results were based on the same reaction equation with the possible exception of CH2. Then, for the above reaction equation, there are four atom-balance equations and the sum of mole fractions identity for six unknowns (again exclude CH2); therefore, an additional constraint is required. For this, the water/gas equilibrium 213 based on the measured local mean temperature and modified as described below, was chosen. Then at various radii in the cross section to give an adequate definition, the reported data were interpolated using cubic splines and the above unknowns computed. Also the asymptotic end of each measured profile was determined from cubic spline fitting (extrapolation). If the above system of equations gave a negative mole fraction of methane (occurring in the high temperature and lean boundary regions) or CO was nonexistent, then the water/gas equilibrium constraint was dropped and the reaction equation solved (excluding both CH_2 and CH_4). Lastly, the outermost regions would not have any free hydrogen (as evidenced by computing negative mole fractions of same). carbon-balance constraint was dropped (taking the ${\rm O}_2$ measurements as being more accurate), and the reaction equation solved for nitrogen, water, and stoichiometry.

The water/gas equilibrium shift results of Mitchell, et al., 129 were applied to the equilibrium constant (determined from measured temperature) in the rich regions of the flame. In the

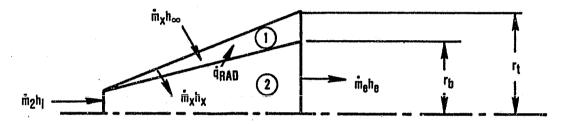
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lean regions at less than 1400°K, the reaction was assumed to be quenched (5) at 1400°K.

With an assumed jet profile of [19],

$$\frac{\mathbf{u}}{\mathbf{u}_{\mathbf{b}}} = \left[1 - \left(\frac{\mathbf{r}}{\mathbf{r}_{\mathbf{b}}}\right)^{3/2}\right]^{2}$$

where the jet radius (r_b) is minimum of the ${\rm CO}_2$ or ${\rm O}_2$ profile asymptote and the centerline velocity is determined by matching the energy flux. For this balance consider the following control volumes,



Continuity gives $\mathring{\mathbf{m}}_{e} = \mathring{\mathbf{m}}_{i} + \mathring{\mathbf{m}}_{x}$, where $\mathring{\mathbf{m}}_{x}$ is the entrainment, and energy gives

$$\hat{\mathbf{m}} \mathbf{i} \left[\mathbf{h}_{\mathbf{i}} + \frac{\mathbf{u}_{\mathbf{i}}^{2}}{2} \right] = \int_{0}^{r_{\mathbf{b}}} \left[\mathbf{h} + \frac{\mathbf{u}^{2}}{2} \right] \mathbf{u} \rho r d \mathbf{r} - \left\{ \int_{0}^{r_{\mathbf{b}}} \mathbf{u} \rho r d \mathbf{r} - \hat{\mathbf{m}} \mathbf{i} \right\} \mathbf{h}_{\infty}$$

where,

r_t - radius of thermal boundary as determined from the temperature profile

q_{rad} - radiation heat transfer outside jet boundary to mass entrained

 ρ - local density

m_i - initial jet mass flux

This procedure was attempted at all four measurement stations. For the first, x/D = 36.2, the energy flux matching gave $u_b = 26.85$ m/s. The other three stations have more enthalpy in the outer boundary region than matching will allow, indicating that temperature measurements there are high.

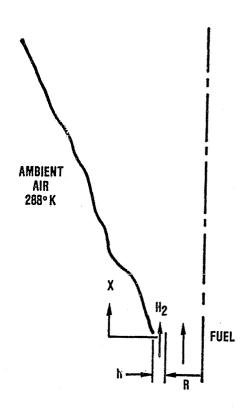
The partial equilibrium computation%s were made with the full stoichiometry adjusted (i.e. amount of CH_{Λ} and N_2) to give the correct enthalpy flux. The 2-D turbulent jet calculations were based on a jet diameter 1 mm larger than that reported (i.e., the OD of the ${\rm H_2}$ stabilizer). Then, an assumed fully developed pipe flow velocity profile at the exit was set to give the correct jet mass flux. 214 The turbulence intensity profile was taken from developed pipe flow results. 215 The partial equilibrium computations were based on the specific thermodynamic of the JANAF tables using the curve fits of Wakelyn and McLain, 216 the three body recombination kinetics of Jensen and Jones²⁸ and the global hydrocarbon breakdown of Duterque, et al. 29 Additionally, the flame sheet approximation had a pyrolysis mixture fraction of 0.073 and 0.2 mass fraction of organic fuel converted to intermediate at the pyrolysis flame sheet. In the 2-D turbulent jet calculations, the initial turbulent length scales were 0.1 inner (jet) and 0.2 outer, both based on the jet diameter. Also the free stream or ambient air was given a velocity of '0.25 m/s.

The axial plots of centerline temperature, CO, CO₂, and O₂ are shown in Figure 6.13-2. The model-predicted centerline temperature profile agrees reasonably well in regard to temperature rise upstream and downstream of the flame tip at the center. The predicted peak temperature level and its axial location are slightly different from data. The initial CO buildup agrees well with data; but there is some discrepancy in the post-flame region. Similar conclusions can be made about the CO₂ profiles shown in Figure

6.13-2. For the initial portion of the flame (x < 0.75 m), measurements indicate finite concentration of O_2 at the centerline. Such a behavior cannot be predicted by diffusion flame models including Bilger's model which, for a high fuel-rich region, sets O_2 equal to zero.

Figure 6.13-3 shows a comparison between measured and predicted profiles of total fuel mass fraction, and unburned fuel profiles are presented in Figure 6.13-4. In the initial portion of the flame, the conclusions are good, but farther down stream the fuel oxidation rate is faster than what data would indicate. This also results in higher centerline temperature levels as shown in Figure 6.13-5. From the model predictions of total fuel mass fraction at x/D = 113.7, it is concluded that the Bilger model is predicting a faster jet spreading rate. This causes faster decay of the centerline temperature in the post-flame region as shown in Figure 6.13-5.

Comparison between measured and predicted CO profiles (Figure 6.13-6) show that, whereas the agreement is good up to x/D = 75, the post-flame region is not well correlated by the Bilger model. Similar conclusions can be made for the H_2 profiles as presented in Figure 6.13-7. For the O_2 profiles, (Figure 6.13-8) up to x/D = 75, the model predictions are reasonable. But further downstream the model is predicting higher spreading rate than measurements suggest. Similar levels of correlations are obtained for CO_2 profiles as shown in Figure 6.13-9.



R = 0.00387 M h = 0.0005 M U_{FUEL} = 39.9 M/S T_{FUEL} = 288° K

Figure 6.13-1. Geometry of the Free Methane Turbulent Jet Flame Test Setup.

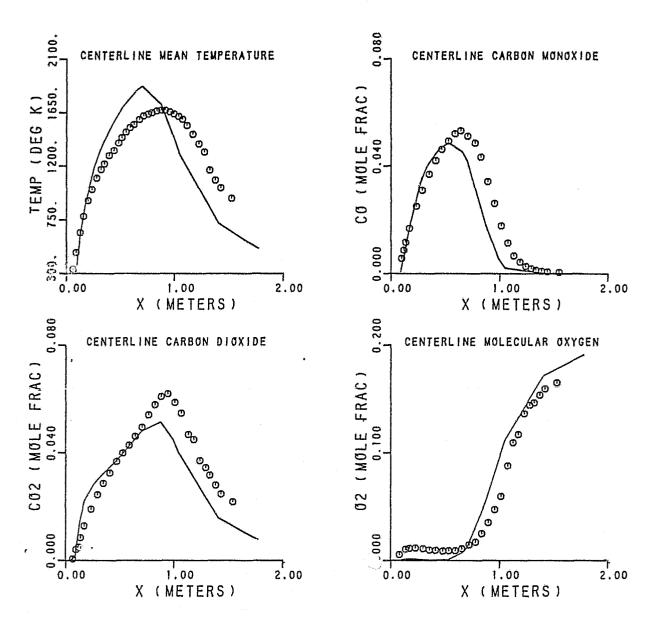


Figure 6.13-2. Comparison Between Bilger Model Predictions With Measured Centerline Profiles of Temperature, CO, CO₂ and O₂ for Hassan and Lockwood Methane Jet Flame.

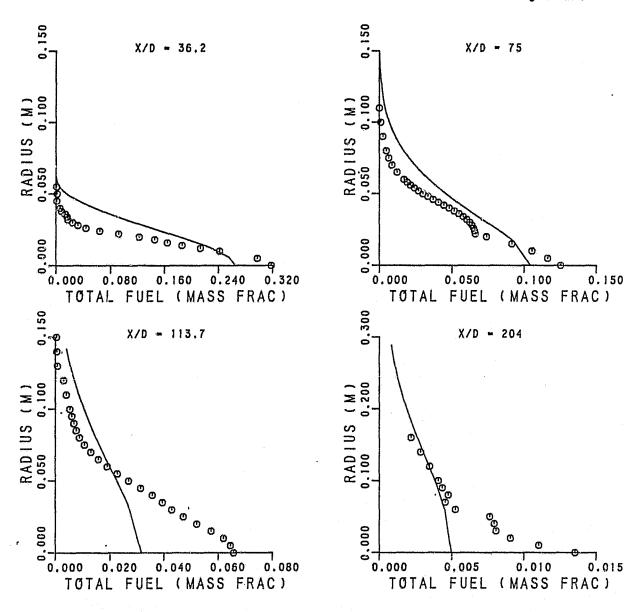
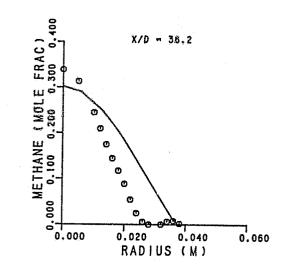


Figure 6.13-3. Radial Profiles of Total Fuel (Bilger's Model).



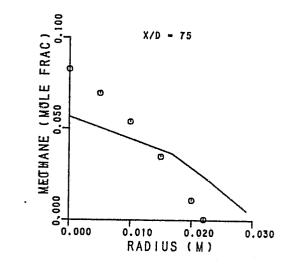


Figure 6.13-4. Radial Profiles of Unburned Fuel Mass Fraction.

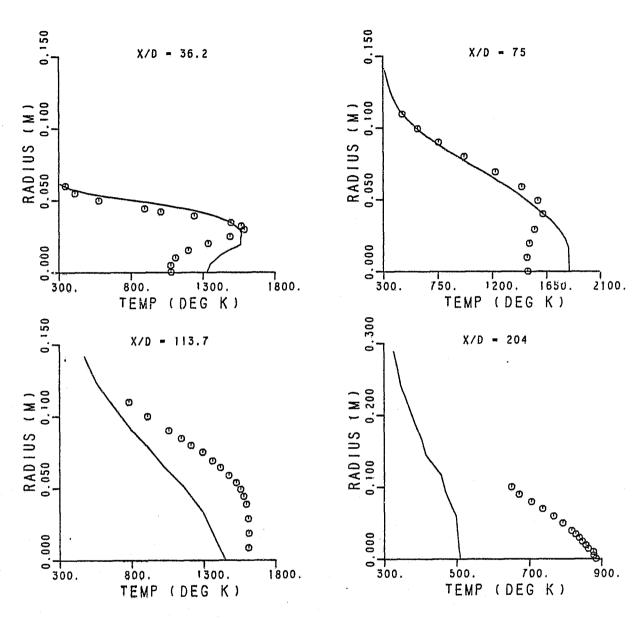
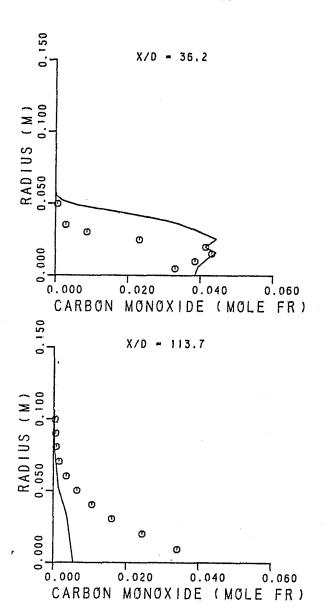


Figure 6.13-5. Radial Profiles of Temperature (Bilger's Model).



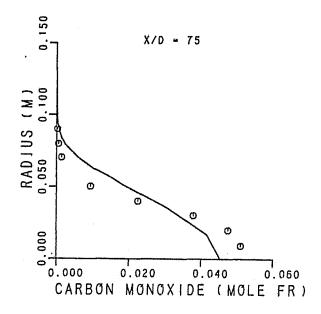


Figure 6.13-6. Radial Profiles of CO (Bilger's Model).

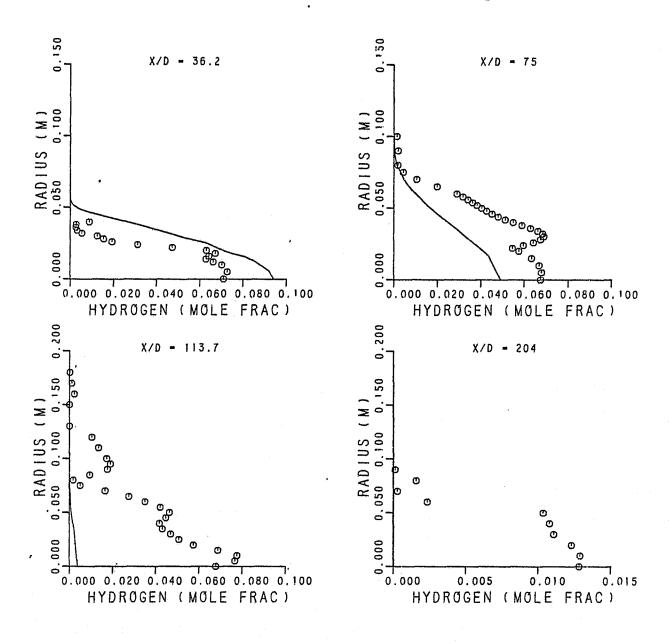


Figure 6.13-7. Radial Profiles of H_2 (Bilger's Model).

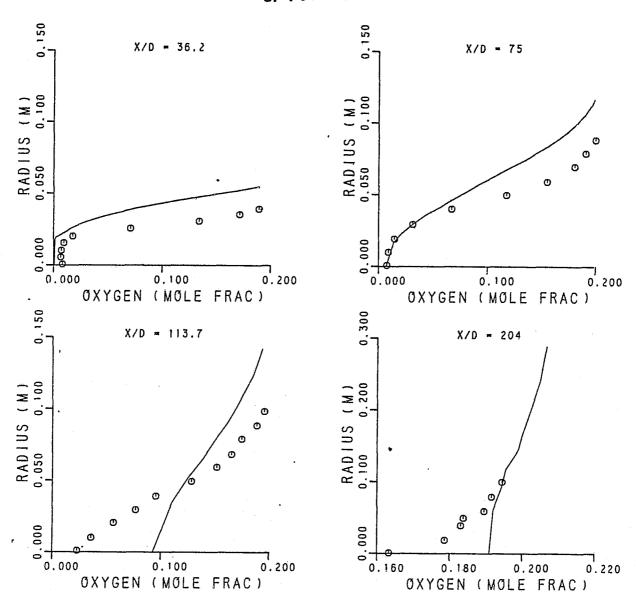


Figure 6.13-8. Radial Profiles of O_2 (Bilger's Model).

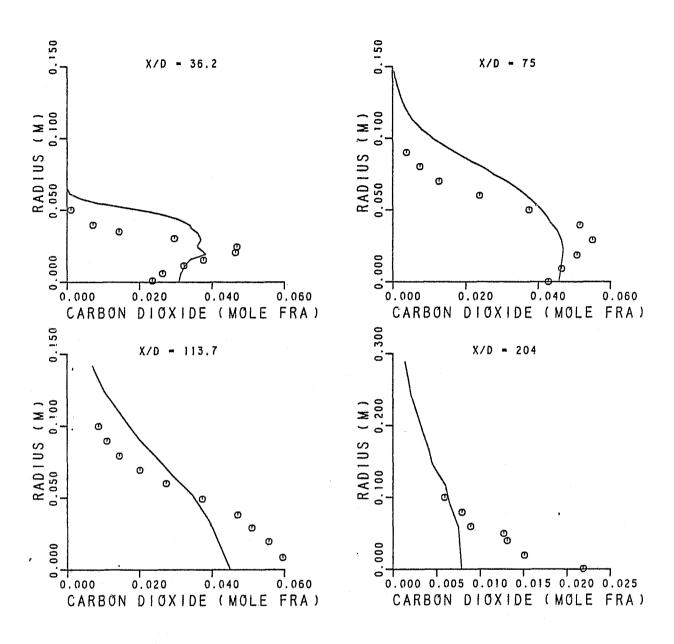


Figure 6.13-9. Radial Profiles of CO₂ (Bilger's Model).